

RESEARCH ARTICLE

Parametrizations of density matrices

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This article gives a brief overview of some recent progress in the characterization and parametrization of density matrices of finite dimensional systems. We discuss in some detail the Bloch-vector and Jarlskog parametrizations and mention briefly the coset parametrization. As applications of the Bloch parametrization we discuss the trace invariants for the case of time dependent Hamiltonians and in some detail the dynamics of three-level systems. Furthermore, the Bloch vector of two-qubit systems as well as the use of the polarization operator basis is indicated. As the main application of the Jarlskog parametrization we construct density matrices for composite systems. In addition, some recent related articles are mentioned without further discussion.

1. Introduction

1.1. Motivation

The state of a quantum system can be mathematically represented as a density matrix, a positive semidefinite hermitian operator of trace one. The density matrices of finite dimensional systems, which are the topic of this review, can be expressed as complex $n \times n$ matrices, constrained by the hermiticity, positivity, and trace conditions. Considering the fundamental role of density matrices for the description of physical systems, it is not surprising that many investigations have been devoted to the parametrizations of density matrices over the last years. This work is motivated by many reasons. For example, a suitably chosen parametrization may considerably simplify solving a specific physical problem, it may help to identify new properties of the system, or it can be used to study the properties of density operators itself. Furthermore, some parametrizations provide a straightforward way to generate positive matrices. When a general expression for a density matrix is needed, the positivity condition is typically the most difficult property to be sure of. Some parametrizations provide a simple way to overcome this problem.

Maybe the best known density matrix parametrization is the Bloch vector parametrization. It was first used to describe the states of a two-level system, but was later extended to higher dimensions. An early review article discussing the properties of the Bloch vector was published by U. Fano in 1957 (1). In the standard approach using hermitian basis matrices, the Bloch vector of an n -level system is a real vector with $n^2 - 1$ components. In a two-level setting, the Bloch vector is a three component vector with length smaller or equal to one. It provides a way to identify the states of a two-level system with the points of a ball of radius one, the pure states corresponding to the surface of the ball. This mapping has found applications in hundreds, if not thousands, of articles. The two-level case will be mentioned in this review only very briefly as the main emphasis is on higher-dimensional extensions of the Bloch vector description. The structure of the set of Bloch vectors corresponding to positive operators becomes very complicated as soon

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as the dimension increases from two to three. This is a consequence of the fact that when $n > 2$ the maximal length of the Bloch vector producing a positive operator depends on the direction of the vector. The complicated nature of this set is visible already in the three-level case (2–4). However, despite the problems associated with the structure of the set of Bloch vectors giving a physical state, the higher dimensional Bloch vector description has found applications in many fields, such as the dynamics of n -level systems. It has been shown that in this context the Bloch vector parametrization helps to identify constants of motions of some quantum optical systems (5–9). Assuming that the Hamiltonian has a specific shape, the time evolution equation for the Bloch vector can be written in a block form. Vector components belonging to different blocks evolve independently of each other, and it turns out that the length of the vector inside each block is time independent (6, 8, 9). There exists also a class of constants of motion known as trace invariants. Unlike the constants of motion mentioned above, trace invariants are independent of the Hamiltonian of the system. The values of these invariants can be related to the components of the Bloch vector (4). Another field where the Bloch vector parametrization has been used during the recent years is that of quantum entanglement. In particular, the entangled states of two qubits have been studied using this approach by various authors, see, for example, (4, 10–18). In the aforementioned applications the Bloch vector is defined in a basis consisting of hermitian operators. This is often a natural choice as it guarantees that the components of the Bloch vector are real. However, it may be preferable to use the polarization (or spherical tensor) operator basis (19, 20) when the angular symmetries of states are important (21). Another possible choice for the basis is the Weyl operator basis (20). As in the case of the hermitian basis, defining the parameter set corresponding to physical states is a complicated problem also when the latter two bases are used.

It is possible to express every $n \times n$ density matrix in terms of a diagonal matrix and an element of the unitary group $U(n)$. This provides a way to parametrize the density matrices if a parametrization of $U(n)$ is known. There exists many such parametrizations, but, depending on the on the problem, one of them may be preferable by providing a better insight or by leading to a reduction of the number of parameters. In general, a parametrization of $U(n)$ has n^2 real parameters. Consequently, the size of the parameter set grows fast as n increases, encouraging to find ways to reduce the number of parameters. Two examples of parametrizations which allow to identify redundant parameters are the Jarlskog parametrization (22–24) and the parametrization presented in (25). These parametrizations have potential applications in quantum information theory, where many quantities and properties of quantum systems are obtained by optimizing the values of some functions over the set of all density matrices. This is the case, for example, when entanglement is quantified (26, 27). Determining the values of entanglement measures leads often to numerically demanding calculations due to the high-dimensional parameter set over which the optimization has to be performed. Finding a parametrization which allows to construct a sufficiently large set of density operators while keeping the parameter set small would simplify his task considerably. The parametrizations discussed in this review are the coset (28) and Jarlskog parametrizations (22–24). The former consists of parametrizing the density matrices in terms of certain cosets in the group $U(n)$, while in the latter approach the elements of $U(N)$ are given recursively, meaning that the elements of $U(N)$ are expressed in terms of the elements of $U(N - 1)$ and a unitary matrix containing the additional parameters needed to describe an element of $U(N)$. With the help of the Jarlskog parametrization it is straightforward to generate matrices which are guaranteed to be positive. Furthermore, this parametrization can be easily extended to composite systems (29).

In addition to these approaches, there is a parametrization of (special) unitary matrices in terms of generalized Euler angles (30, 31). It has been applied in (31) to derive a volume formula for $U(N)$ and related groups. This parametrization allows to eliminate redundant global phases in several cases. Yet another way to parametrize the elements of $U(N)$ is in terms of quantum Householder reflections (32). This approach has been shown to be useful in quantum computation and quantum state manipulation (32–34). It seems, however, that these two parametrizations of

the unitary group have not been used to parametrize density matrices. Consequently they will not be discussed in more detail in this article. Another related factorization of unitary matrices in terms of orthogonal matrices is described in (35). A substantial generalization of these ideas can be found in (36).

1.2. Basic definitions

Recall that in quantum physics states are represented by density matrices on the complex Hilbert space \mathcal{H} of the system. The Hilbert space \mathcal{H} is always separable and in many cases of modern applications actually finite dimensional.

A *density matrix* ρ on a Hilbert space \mathcal{H} is by definition a linear operator from \mathcal{H} into \mathcal{H} such that

$$\rho \geq 0 \text{ i.e., } \langle x, \rho x \rangle \geq 0 \text{ for all } x \in \mathcal{H} \quad (1)$$

and

$$\text{Tr}(\rho) = \sum_{j=1}^{\infty} \langle e_j, \rho e_j \rangle = 1, \quad (2)$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product of the Hilbert space \mathcal{H} , $\{e_j : j \in \mathbb{N}\}$ is any orthonormal basis of \mathcal{H} and the normalization condition for the trace is written for the infinite dimensional case. In this case one has also to assume that ρ is of trace class. If \mathcal{H} is of finite dimension n , then the sum in (2) extends from $j = 1$ to $j = n$.

In this article we consider the case where the Hilbert space \mathcal{H} is n -dimensional, $n \in \mathbb{N}$,

$$\mathcal{H} = \mathcal{H}_n = \mathbb{C}^n. \quad (3)$$

We denote the basis of \mathbb{C}^n by $\{|1\rangle, |2\rangle, \dots, |n\rangle\}$. Now linear operators A on \mathcal{H} are represented by $n \times n$ matrices with complex entries, and in the following we do not distinguish between a matrix and the linear operator it represents. We denote by \mathcal{M}_n the space of all $n \times n$ matrices with complex entries. Then a density matrix ρ on \mathcal{H}_n is an element $\rho \in \mathcal{M}_n$ such that the positivity condition (1) and the normalization condition (2) for the trace hold.

It is well known (and straightforward to prove) that in a complex Hilbert space a linear operator A which is positive in the sense of (1) (often also called positive semi-definite) is Hermitian, i.e., it satisfies $A = A^*$, where A^* is the adjoint matrix defined by

$$(A^*)_{ij} = \bar{a}_{ji} \text{ for all } i, j = 1, \dots, n \quad (4)$$

Here a_{ij} are the coefficients of the matrix A and \bar{a}_{ji} denotes the complex conjugate of a_{ji} .

The eigenvalues of a matrix $A \geq 0$ (i.e., A satisfies (1)) are calculated as follows (see, for instance, Theorem 25.1.1 of (37)): The first eigenvalue is given by

$$\lambda_1 = \sup\{\langle x, Ax \rangle : x \in \mathcal{H}_n, \|x\| = 1\}, \quad (5)$$

and one proves easily from this definition that there is a vector $e_1 \in \mathcal{H}_n$, $\|e_1\| = 1$ such that $Ae_1 = \lambda_1 e_1$. The second eigenvalue then is $(\{e_1\}^\perp)$ denotes the orthogonal complement of $\{e_1\}$ in \mathcal{H}_n)

$$\lambda_2 = \sup\{\langle x, Ax \rangle : x \in \{e_1\}^\perp \subset \mathcal{H}_n, \|x\| = 1\}, \quad (6)$$

and there is $e_2 \in \{e_1\}^\perp$, $\|e_2\| = 1$ such that $Ae_2 = \lambda_2 e_2$. This procedure can be iterated and produces eigenvalues

$$\lambda_1, \dots, \lambda_n; \quad \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0. \quad (7)$$

These n eigenvalues are not necessarily distinct; they occur in this list as many times as their multiplicity requires. For the eigenvalues of a matrix $A \geq 0$ with $\text{Tr}(A) = 1$ we know in addition to (7) that

$$\lambda_1 > 0 \quad \text{and} \quad \sum_{j=1}^n \lambda_j = 1. \quad (8)$$

We know that the system of eigenvectors e_1, \dots, e_n of A is a complete orthogonal system in \mathcal{H}_n . Therefore, the transition from the standard basis of \mathcal{H}_n to the basis of eigenvectors is effected by a unitary $n \times n$ matrix U , and we arrive at the *spectral representation* of the matrix A :

$$A = U^* D_n(\lambda_1, \dots, \lambda_n) U, \quad (9)$$

with

$$D_n(\lambda_1, \dots, \lambda_n) = \begin{pmatrix} \lambda_1 & 0 & 0 & \cdots & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \lambda_{n-1} & 0 \\ 0 & \cdots & 0 & 0 & \lambda_n \end{pmatrix} \quad (10)$$

being the diagonal matrix of eigenvalues.

Thus a density matrix can be characterized as follows:

A matrix $\rho \in \mathcal{M}_n^h$ (\mathcal{M}_n^h denotes the space of all Hermitian elements of \mathcal{M}_n) with coefficients $\rho_{ij} \in \mathbb{C}$, $i, j = 1, \dots, n$ is a *density matrix* if, and only if,

(a) ρ is positive in the sense of (1), i.e. all eigenvalues λ_j are nonnegative,

$$\lambda_j = \lambda_j(\rho) \geq 0 \quad \text{for } j = 1, \dots, n; \quad (11)$$

(b)

$$\text{Tr}(\rho) = \sum_{j=1}^n \rho_{jj} = 1. \quad (12)$$

Let us introduce the set \mathcal{D}_n of all n -dimensional density matrices,

$$\mathcal{D}_n = \{\rho \in \mathcal{M}_n^h : \rho \text{ satisfies (11) and (12)}\}. \quad (13)$$

In this article we study the general form of the elements of \mathcal{D}_n . The main difficulty is the positivity constraint $\rho \geq 0$. There are a number of criteria a matrix has to satisfy for positivity. Since they are typically given in terms of inequalities they do not provide much information about the concrete form of a density matrix.

In this article we review recent studies on the structure and general form of a density matrix. Ideally one would like to have a parametrization of density matrices in the following sense: A *parametrization of a density matrix* $\rho \in \mathcal{D}_n$ means the following:

(a) Specification of a parameter set $Q_n \subset \mathbb{R}^m$ where m depends on n , i.e., $m = m(n)$;

(b) Specification of a one-to-one and onto map $F_n : Q_n \longrightarrow \mathcal{D}_n$.

Clearly, the case $n = 1$ is trivial: $\mathcal{D}_1 = \{1\}$. Therefore in the following we assume $n \geq 2$.

Unfortunately, this type of a parametrization of density matrices is not yet available for general $n \geq 3$. Only the case $n = 2$ is fully understood. We discuss here the partial results of the three main approaches to this problem:

- the Bloch-vector parametrization;
- the coset parametrization;
- the Jarlskog parametrization.

1.3. Overview

Although the case $n = 2$ has been studied a lot in the literature, we start the following section on the Bloch-vector parametrization with a review of this case. This serves as a preparation for the discussion on the general case $n \geq 3$. This discussion is based mostly on (3, 4) and it provides a reference point for the representations presented in sections 3 and 4, where it turns out that all parametrizations agree for $n = 2$, but not for $n > 2$. We show that, despite the fact that the determination of the parameter set Q_n is a difficult task, the Bloch-vector parametrization can be used to identify various constants of motion or to study the properties of two-qubit states.

Obviously, the spectral representation (9) can be used to obtain a parametrization of density matrices as soon as a parametrization of unitary matrices is known. Several parametrizations of unitary matrices can be found in the literature. We mention those which are of interest in connection with our problem of parametrizing density matrices. One of them is the coset parametrization (see, for instance, (38)). It has been used in (39) as a starting point for an analysis of the space of all density matrices for $n = 4$. This analysis gives a description of the geometry of this state space in terms of flag manifolds. However, no parametrization of individual density matrices is offered. This idea has later been used in (28) to propose a parametrization of density matrices in terms of certain cosets in the group $U(n)$. Section 3 contains a brief summary and discussion about the extent to which this parametrization can be considered a parametrization in the sense given above.

The next section introduces the Jarlskog parametrization (see (40)). This parametrization is closely related to the coset parametrization and again starts from the spectral representation (9) but uses the parametrization of $U(n)$ presented by Jarlskog (see (22, 24)) instead of cosets. The Jarlskog parametrization is recursive and thus allows a recursive parametrization of density matrices. We apply the Jarlskog parametrization to composite systems and obtain several quite interesting cases of a parametrization of density matrices for composite systems (29). Finally, section 5 contains the concluding remarks.

2. Bloch-vector parametrization

In this section we first describe the Bloch vector of a two-level system, and then extend the discussion to n -dimensional systems. We show what is required from the Bloch vector of a three-level system for it to describe a physical state. We illustrate the use of the Bloch vector in identifying constants of motion of dynamical systems, and then show how the Bloch vector approach can be used to study the separability of a two-qubit system. We also briefly describe an alternative basis for the Bloch vector parametrization, known as the polarization operator basis.

2.1. The case $n = 2$: The Bloch/Poincaré sphere

It is not difficult to see that the Pauli matrices

$$\sigma_x = \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (14)$$

together with the identity matrix I_2 form a basis of the real vector space \mathcal{M}_2^h of Hermitian 2×2 matrices. Hence every $A \in \mathcal{M}_2^h$ can be represented as

$$A = a_0 I_2 + \lambda_1 \sigma_1 + \lambda_2 \sigma_2 + \lambda_3 \sigma_3,$$

where a_0 and λ_j , $j = 1, 2, 3$ are real numbers. Since the trace of the Pauli matrices vanishes, the coefficient a_0 is determined by $\text{Tr}(A) = 2a_0$. Hence, such a matrix belongs to \mathcal{D}_2 if and only if it has a representation

$$A = \frac{1}{2} I_2 + \frac{1}{2} \sum_{j=1}^3 \lambda_j \sigma_j = \frac{1}{2} \begin{pmatrix} 1 + \lambda_3 & \lambda_1 - i\lambda_2 \\ \lambda_1 + i\lambda_2 & 1 - \lambda_3 \end{pmatrix}, \quad (15)$$

in which the coefficients λ_j are chosen such that all the eigenvalues of A are non-negative. The eigenvalues of A can be calculated by finding the roots of the characteristic polynomial $\det(xI_2 - A)$. Using the abbreviation $\lambda'_j = \frac{1}{2}\lambda_j$ we find for this polynomial ($\underline{\lambda} = (\lambda_1, \lambda_2, \lambda_3) \in \mathbb{R}^3$ and $|\underline{\lambda}|^2 = \sum_{j=1}^3 \lambda_j^2$)

$$\det(xI_2 - A) = \left(x - \frac{1}{2}\right)^2 - |\underline{\lambda}'|^2 = x^2 - x + \frac{1}{4} - |\underline{\lambda}'|^2. \quad (16)$$

The roots of this polynomial are

$$x_1 = \frac{1}{2}(1 + |\underline{\lambda}|) \quad \text{and} \quad x_2 = \frac{1}{2}(1 - |\underline{\lambda}|). \quad (17)$$

While the root x_1 is always $\geq \frac{1}{2}$, the root x_2 is non-negative if and only if $|\underline{\lambda}| \leq 1$. This gives our first result: The parameter set for this case is

$$Q_2 = \{\underline{\lambda} \in \mathbb{R}^3 : |\underline{\lambda}| \leq 1\} = B(\mathbb{R}^3), \quad (18)$$

where $B(\mathbb{R}^3)$ denotes the closed unit ball in \mathbb{R}^3 with center at 0. We define a map on Q_2 with values in \mathcal{D}_2 by the right hand side of (15), i.e.,

$$F_2(\underline{\lambda}) = \frac{1}{2} \begin{pmatrix} 1 + \lambda_3 & \lambda_1 - i\lambda_2 \\ \lambda_1 + i\lambda_2 & 1 - \lambda_3 \end{pmatrix}, \quad \underline{\lambda} \in Q_2. \quad (19)$$

By construction, this map is onto \mathcal{D}_2 . A simple argument shows that F_2 is also one-to-one, i.e., $F_2(\underline{\lambda}) = F_2(\underline{\lambda}')$ implies $\underline{\lambda} = \underline{\lambda}'$. We conclude that that (Q_2, F_2) is a parametrization of \mathcal{D}_2 with $m = 3 = n^2 - 1$ for $n = 2$.

The parameter set $Q_2 = B(\mathbb{R}^3)$ in this parametrization of \mathcal{D}_2 is called the *Bloch* or *Poincaré ball*. In order to relate it to the standard representation and interpretation we just have to introduce spherical polar coordinates in $B(\mathbb{R}^3)$:

$$\lambda_1 = r \sin \theta \cos \phi, \quad \lambda_2 = r \sin \theta \sin \phi, \quad \lambda_3 = r \cos \theta, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \phi < 2\pi, \quad 0 \leq r \leq 1. \quad (20)$$

Using the spherical coordinates we can introduce a new parameter set

$$\tilde{Q}_2 = \{(\theta, \phi, r) \in \mathbb{R}^3 : 0 \leq \theta \leq \pi, 0 \leq \phi < 2\pi, 0 \leq r \leq 1\} \quad (21)$$

and on it the map \tilde{F}_2 with values in \mathcal{D}_2 , defined by

$$\tilde{F}_2(\theta, \phi, r) = F_2(\underline{\lambda}(\theta, \phi, r)) = \begin{pmatrix} \frac{1}{2}(1 + r \cos \theta) & \frac{r}{2}e^{-i\phi} \sin \theta \\ \frac{r}{2}e^{i\phi} \sin \theta & \frac{1}{2}(1 - r \cos \theta) \end{pmatrix}, \quad (\theta, \phi, r) \in \tilde{Q}_2. \quad (22)$$

The boundary of the Bloch/Poincaré ball is called the *Bloch/Poincaré sphere*. In terms of the parameter sets Q_2 and \tilde{Q}_2 this sphere is given by $|\underline{\lambda}| = 1$ and $r = 1$, respectively. Introducing the angle $\vartheta = \theta/2$ and using some elementary relations for the trigonometric functions \sin and \cos , the pure state density matrix corresponding to the point $(\theta, \phi, 1)$ on the Bloch/Poincaré sphere has the form

$$\tilde{F}_2(2\vartheta, \phi, 1) = \begin{pmatrix} c^2 & cse^{-i\phi} \\ cse^{i\phi} & s^2 \end{pmatrix} = |\psi\rangle\langle\psi|, \quad (23)$$

where we used the abbreviations $c = \cos \vartheta$ and $s = \sin \vartheta$, and

$$|\psi\rangle = (c, se^{i\phi})^T = \cos \vartheta |0\rangle + e^{i\phi} \sin \vartheta |1\rangle. \quad (24)$$

2.2. The general case $n \geq 3$

As the last subsection shows, the Bloch vector parametrization works quite well in the case of 2-level systems ($n = 2$). It has been generalized to the case of n -level systems with $n \geq 3$. The starting point of this generalization is the observation that the Pauli-matrices in (15) can be considered as the generators of the special unitary group $SU(2)$. Therefore the following representation of density matrices $\rho \in \mathcal{D}_n$ has been suggested:

$$\rho = \frac{1}{n}I_n + \frac{1}{2} \sum_{j=1}^{n^2-1} \lambda_j \hat{\lambda}_j, \quad (25)$$

where $\hat{\lambda}_j$, $j = 1, \dots, n^2 - 1$, are the (orthogonal) generators of the special unitary group $SU(n)$ and the λ_j , $j = 1, \dots, n^2 - 1$, are real numbers. The generators $\hat{\lambda}_j$ are $n \times n$ matrices with complex coefficients satisfying

$$\hat{\lambda}_j^* = \hat{\lambda}_j, \quad \text{Tr} \hat{\lambda}_j = 0, \quad \text{Tr}(\hat{\lambda}_i \hat{\lambda}_j) = 2\delta_{ij}, \quad i, j = 1, \dots, n^2 - 1 \quad (26)$$

and the commutation and anti-commutation relations

$$[\hat{\lambda}_i, \hat{\lambda}_j] = 2i \sum_{k=1}^{n^2-1} f_{ijk} \hat{\lambda}_k, \quad [\hat{\lambda}_i, \hat{\lambda}_j]_+ = \frac{4}{n} \delta_{ij} I_n + 2 \sum_{k=1}^{n^2-1} g_{ijk} \hat{\lambda}_k. \quad (27)$$

Here the f_{ijk} and g_{ijk} are the structure constants of the Lie algebra $su(n)$. It is also known that the generators $\hat{\lambda}_i$, $i = 1, \dots, n^2 - 1$ together with the unit matrix I_n form an orthogonal basis of \mathcal{M}_n^h with respect to the Hilbert-Schmidt inner product $\langle A, B \rangle = \text{Tr}(A^* B)$. This means that the inner product of two density matrices ρ and $\tilde{\rho}$, with Bloch vectors $\underline{\lambda}$ and $\tilde{\underline{\lambda}}$, reads simply $\langle \rho, \tilde{\rho} \rangle = \underline{\lambda} \cdot \tilde{\underline{\lambda}}$.

The vector $\underline{\lambda}$ is in this review called Bloch vector. In order to make a difference between the Bloch vector of a two-level system and that of an n -level system, $n > 2$, the term *generalized*

Bloch vector is sometimes used in the literature to describe the latter case. Yet another possible name for the Bloch vector is *coherence vector*.

One possible explicit construction for the generators $\hat{\lambda}_j$ can be given in terms of the generalized Gell-Mann matrices by defining the basis as in the following equation.

$$\begin{aligned} &|j\rangle\langle k| + |k\rangle\langle j|, & 1 \leq j < k \leq n, \\ &-i|j\rangle\langle k| + i|k\rangle\langle j|, & 1 \leq j < k \leq n, \\ &\sqrt{\frac{2}{l(l+1)}} \left(\sum_{j=1}^l |j\rangle\langle j| - l|l+1\rangle\langle l+1| \right), & 1 \leq l \leq n-1. \end{aligned} \quad (28)$$

If $n = 2$ these correspond to the Pauli matrices (14) and if $n = 3$ they are the Gell-Mann matrices, see (49) below.

According to the properties (26) of the generators $\hat{\lambda}_j$ every matrix of the form (25) has trace 1, $\text{Tr} \rho = 1$. Thus a matrix of the form (25) is a density matrix if and only if all its eigenvalues are non-negative. As in the case $n = 2$ these eigenvalues are the roots of the characteristic polynomial $\det(xI_n - \rho)$. As a polynomial of degree n the characteristic polynomial has a unique representation of the form

$$\det(xI_n - \rho) = \sum_{j=0}^n (-1)^j a_j x^{n-j}, \quad a_0 = 1, \quad (29)$$

where the coefficients a_j are uniquely determined by the generators $\hat{\lambda}_j$ and the parameters $\underline{\lambda} = (\lambda_1, \dots, \lambda_{n^2-1}) \in \mathbb{R}^{n^2-1}$. In order to emphasize the dependence on $\underline{\lambda}$ we write $a_j = a_j(\underline{\lambda})$.

If x_1, \dots, x_n denote the roots of the characteristic polynomial $\det(xI_n - \rho)$, then (29) shows

$$\sum_{j=0}^n (-1)^j a_j x^{n-j} = \prod_{j=1}^n (x - x_j) \quad (30)$$

and by evaluating the product and comparing coefficients, the basic relation between the coefficients a_j and the roots x_j follows:

$$a_j = \sum_{1 \leq i_1 < i_2 < \dots < i_j} x_{i_1} x_{i_2} \dots x_{i_j} \quad \text{Vieta's formula.} \quad (31)$$

It is known (an elementary proof is given in the appendix of (3)) that from this formula the important characterization of the non-negativity of the eigenvalues follows:

$$x_j \geq 0, \quad j = 1, \dots, n, \quad \Leftrightarrow \quad a_j \geq 0, \quad j = 1, \dots, n. \quad (32)$$

Accordingly we define the parameter set as Q_n

$$Q_n = \{\underline{\lambda} \in \mathbb{R}^{n^2-1} : a_j(\underline{\lambda}) \geq 0, \quad j = 1, \dots, n\}, \quad (33)$$

and on Q_n the map $F_n : Q_n \longrightarrow \mathcal{D}_n$ by

$$F_n(\underline{\lambda}) = \frac{1}{n} I_n + \frac{1}{2} \sum_{j=1}^{n^2-1} \lambda_j \hat{\lambda}_j, \quad \underline{\lambda} \in Q_n. \quad (34)$$

The inverse of this map is given by

$$F_n^{-1}(\rho) = (\lambda_1 = \text{Tr}(\rho \hat{\lambda}_1), \dots, \lambda_{n^2-1} = \text{Tr}(\rho \hat{\lambda}_{n^2-1})), \quad \rho \in \mathcal{D}_n. \quad (35)$$

Thus, (Q_n, F_n) is a parametrization for n -level density matrices $\rho \in \mathcal{D}_n$. It is called the *Bloch-vector parametrization*.

Now we discuss the difficulties with this parametrization for concrete applications. Although the parameter set Q_n is uniquely specified, it is not easy to decide when a given point $\underline{\lambda} \in \mathbb{R}^{n^2-1}$ actually belongs to Q_n . The origin of this difficulty is that firstly it is quite a complicated matter to explicitly calculate the coefficients a_j for larger values of j and secondly it is not easy to determine explicitly the boundary of Q_n , i.e., the set $\partial Q_n = \{\underline{\lambda} \in \mathbb{R}^{n^2-1} : a_j(\underline{\lambda}) = 0, j = 1, \dots, n^2 - 1\}$ since this amounts to solving polynomial equations in $\underline{\lambda}$ of degree n , in $n^2 - 1$ variables.

Using Lie algebra techniques, the polynomials $a_j(\underline{\lambda})$, $j = 1, 2, 3, 4$, have been calculated explicitly in (3) (see also (4)). They read as follows:

$$\begin{aligned} 1!a_1 &= 1, \\ 2!a_2 &= \left(\frac{n-1}{n} - \frac{1}{2}|\underline{\lambda}|^2 \right), \\ 3!a_3 &= \left[\frac{(n-1)(n-2)}{n^2} - \frac{3(n-2)}{2n}|\underline{\lambda}|^2 + \frac{1}{2} \sum_{i,j,k=1}^{n^2-1} g_{ijk} \lambda_i \lambda_j \lambda_k \right], \\ 4!a_4 &= \left[\frac{(n-1)(n-2)(n-3)}{n^3} - \frac{3(n-2)(n-3)}{n^2}|\underline{\lambda}|^2 + \frac{3(n-2)}{4n}|\underline{\lambda}|^4 \right. \\ &\quad \left. + \frac{2(n-3)}{n} \sum_{i,j,k=1}^{n^2-1} g_{ijk} \lambda_i \lambda_j \lambda_k - \frac{3}{4} \sum_{i,j,k,l,p=1}^{n^2-1} g_{ijk} g_{klp} \lambda_i \lambda_j \lambda_l \lambda_p \right]. \end{aligned} \quad (36)$$

Already for $n = 3$ the parameter set has not been determined explicitly though $a_3(\underline{\lambda})$ is known. If in (36) we insert the explicit values of the structure constants g_{ijk} for the chosen set of generators of $su(3)$, a_3 is given by (recall that $n^2 - 1$ is 8 for $n = 3$)

$$\begin{aligned} 3!a_3(\underline{\lambda}) &= \frac{1}{36} \left\{ 8 - 18|\underline{\lambda}|^2 + 27\lambda_3(\lambda_4^2 + \lambda_5^2 - \lambda_6^2 - \lambda_7^2) - 6\sqrt{3}\lambda_8^3 \right. \\ &\quad \left. + 9\sqrt{3}\lambda_8[2(\lambda_1^2 + \lambda_2^2 + \lambda_3^2) - (\lambda_4^2 + \lambda_5^2 + \lambda_6^2 + \lambda_7^2)] + 54(\lambda_1\lambda_4\lambda_6 + \lambda_1\lambda_5\lambda_7 + \lambda_2\lambda_5\lambda_6 - \lambda_2\lambda_4\lambda_7) \right\} \end{aligned} \quad (37)$$

Thus it is obvious that the set $a_3(\underline{\lambda}) \geq 0$ and with it the parameter set Q_3 has not been determined explicitly. However in (3) some 2-dimensional sections have been calculated and represented graphically¹. They show the very complicated nature of these sets.

The Bloch vector parametrization has found applications in many different fields: It was used extensively by Harriman to study the properties of density operators (2, 41–43). In particular, he discussed the structure of the set of physical states Q_n (2). This work was later extended, and partly reproduced, by other authors (3, 4). It has been useful in studying the dynamics and constants of motions of n -level systems (5–9, 44, 45), Markovian dynamics of decaying two-level systems (46–48), entropy production (49), characterization of the reachable sets for open systems driven by unitary control (50), and unitary orbits in the set of density operators (51).

¹We remark that equation (31) of (3) contains typing errors. The correct expression is given by (37) above.

Furthermore, it has been used in studying the properties of two- and n - qubit systems (4, 10–17), the geometry of the states of a finite-dimensional systems (52), the classification of density matrices into different types (53, 54), detecting the entanglement properties of bipartite quantum states (55), characterizing the structure of the state space of a two-qubit system (56) and the steady states of open quantum systems (57).

In the following we briefly discuss some of these applications.

2.3. Bloch parametrization and trace invariants

As we show next, n -level systems can be associated with constants of motion which are independent of the form of the Hamiltonian and depend only on the initial state of the system. These constants of motion are obtained by tracing over ρ^n , $n = 1, 2, \dots$, and are therefore called trace invariants. These invariants can be expressed using the Bloch vector and their values are also related to the coefficients a_i of the polynomial (30) (3, 4). The following discussion is based on (3, 4, 6).

Before introducing the trace invariants, we derive the differential equation that determines the time-evolution of the Bloch vector. The time-evolution of an n -level system can be expressed in terms of its density matrix ρ which satisfies the Liouville equation

$$i \frac{d\rho(t)}{dt} = [\hat{H}(t), \rho(t)], \quad (38)$$

where the Hamiltonian \hat{H} is in general time dependent and we have set $\hbar = 1$. It has been shown in (58) (see also (59, 60)) that under certain conditions for the Hamiltonian² this equation can be solved in the form

$$\rho(t) = U_t \rho(0) U_t^* \quad (39)$$

where U_t , $t \in \mathbb{R}$, is a family of unitary operators (which in general is neither a group nor a semi-group) and where $\rho(0)$ is the initially given density matrix at time $t = 0$. This form of the time evolution guarantees that one stays in the space of density matrices. We write ρ as in (25)

$$\rho = \frac{1}{n} I_n + \frac{1}{2} \sum_{j=1}^{n^2-1} \lambda_j \hat{\lambda}_j. \quad (40)$$

Here and in what follows the time-dependence of the states and Hamiltonians is not always explicitly indicated. The Hamiltonian \hat{H} can be expressed in a similar way

$$\hat{H} = \frac{h_0}{n} I_n + \frac{1}{2} \sum_{i=1}^{n^2-1} h_i \hat{\lambda}_i, \quad (41)$$

where

$$h_0 = \text{Tr} \hat{H}, \quad h_j = \text{Tr}(\hat{\lambda}_j \hat{H}), \quad j = 1, \dots, n^2 - 1. \quad (42)$$

Using (40), (41) and the Liouville equation, the following equation for the time-evolution of the

² $H(t)$ is bounded and self-adjoint and the map $t \mapsto H(t)$ is strongly continuous

Bloch vector can be obtained

$$\frac{d\lambda_i}{dt} = \sum_{j,k=1}^n f_{ijk} h_j \lambda_k. \quad (43)$$

The structure constant f_{ijk} is antisymmetric, which guarantees that the length of $\underline{\lambda}$ is time independent. In addition to this constant of motion, also other conserved quantities can be easily identified. We denote the rank of ρ by r . Then the density matrix can be associated with r constants of motion, as can be seen by writing the density matrix at instant t as

$$\rho(t) = V(t) D V^*(t), \quad D = D_n(\mu_1, \mu_2, \dots, \mu_n), \quad (44)$$

where D is a diagonal matrix of the eigenvalues of ρ and V is a map $V : \mathbb{R} \rightarrow U(n)$. The eigenvalues are time independent and V gives the time-evolution of the state. Now

$$\text{Tr}(\rho^k(t)) = \text{Tr}(D^k) = \mu_1^k + \mu_2^k + \dots + \mu_n^k \quad (45)$$

defines a constant of motion for each integer $k > 0$. The number of non-zero eigenvalues is equal to the rank of ρ , so there are r independent constants of motion, given by $\text{Tr}(\rho^k)$, $k = 1, 2, \dots, r$. Due to the way they are defined, these constants are called trace invariants. Instead of using (44), it is possible to prove the existence of the trace invariants using (43) and the properties of the generators $\{\hat{\lambda}_j\}$ of $SU(n)$. The values of the trace invariants can be expressed in terms of the Bloch vector $\underline{\lambda}$. For $k = 1, 2, 3, 4$ they are

$$\begin{aligned} \text{Tr} \rho &= 1 \\ \text{Tr}(\rho^2) &= \frac{1}{n} + \frac{1}{2} |\underline{\lambda}|^2 \\ \text{Tr}(\rho^3) &= \frac{1}{n^2} + \frac{3}{2n} |\underline{\lambda}|^2 + \frac{1}{4} \underline{\lambda} \cdot (\underline{\lambda} \odot \underline{\lambda}) \\ \text{Tr}(\rho^4) &= \frac{1}{n^3} + \frac{3}{n^2} |\underline{\lambda}|^2 + \frac{1}{n} \underline{\lambda} \cdot (\underline{\lambda} \odot \underline{\lambda}) + \frac{1}{4n} |\underline{\lambda}|^4 + \frac{1}{8} |\underline{\lambda} \odot \underline{\lambda}|^2, \end{aligned} \quad (46)$$

where we have defined

$$(\underline{a} \odot \underline{b})_k = \sum_{i,j=1}^{n^2-1} g_{ijk} a_i b_j. \quad (47)$$

Explicit formulas for the trace invariants for $n = 1, \dots, 9$ given in terms of the Bloch vector can be found in the Appendix B of (4). Conditions for a vector $\underline{\lambda}$ to describe a pure state can be obtained from these equations by setting $\text{Tr}(\rho^k) = 1$. In this way one also obtains the boundary ∂Q_n of Q_n , which consists of pure states.

Comparing (36) and (46) we see that the coefficients a_i can be given in terms of the trace

invariants. The expressions for the first four coefficients and the general expression are

$$\begin{aligned}
 1!a_1 &= \text{Tr}\rho = 1 \\
 2!a_2 &= 1 - \text{Tr}(\rho^2) \\
 3!a_3 &= 1 - 3\text{Tr}(\rho^2) + 2\text{Tr}(\rho^3) \\
 4!a_4 &= 1 - 6\text{Tr}(\rho^2) + 8\text{Tr}(\rho^3) - 6\text{Tr}(\rho^4) + 3\text{Tr}(\rho^2)^2 \\
 k!a_k &= (k-1)! \left((-1)^{k-1} \text{Tr}(\rho^k) + \sum_{i=1}^{k-1} (-1)^{i-1} \text{Tr}(\rho^i) a_{k-i} \right). \tag{48}
 \end{aligned}$$

Clearly also the coefficients a_i are time independent. With the help of (46) these can be expressed using the Bloch vector.

2.4. Bloch parametrization and the dynamics of three-level systems

We now describe how the Bloch vector parametrization can be used to study the dynamics of three-level systems. This topic was studied long before the structure of the set Q_n , that is, the structure of the set of Bloch vectors corresponding to physical states, was examined. We remark that in these studies it was not necessary to know the exact shape of the set Q_n . This is a consequence of the unitary time-evolution, which guarantees that the Bloch vector $\underline{\lambda}(t)$ belongs to the set Q_n at all times $t > 0$ if it is an element of Q_n at $t = 0$. One has only to make sure that the initial state determined by $\underline{\lambda}(0)$ is a positive operator.

Here and in what follows the initial time is chosen to be $t = 0$. The following discussion is based on (5-9, 44). It was found in (5-7) that the Bloch vector representation of the density matrices allows to identify, in addition to the trace invariants whose values do not depend on the shape of the Hamiltonian, also additional conserved quantities which exist only when the Hamiltonian has a specific form. We illustrate this by studying a three-level system, so the relevant Lie algebra is that of $SU(3)$. One common realization for the basis elements $\{\hat{\lambda}_1, \dots, \hat{\lambda}_8\}$ of this Lie algebra is given by the Gell-Mann matrices:

$$\begin{aligned}
 \hat{\lambda}_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{\lambda}_2 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, & \hat{\lambda}_3 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \\
 \hat{\lambda}_4 &= \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{\lambda}_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, & \hat{\lambda}_6 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\
 \hat{\lambda}_7 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, & \hat{\lambda}_8 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}. \tag{49}
 \end{aligned}$$

The physical system we are interested in consists of a three-level atom interacting with two lasers. The energies of the three atomic levels are ω_1, ω_2 and ω_3 and the energy differences needed now are denoted by $\omega_{12} = \omega_1 - \omega_2$ and $\omega_{23} = \omega_2 - \omega_3$. The frequencies of the two lasers are ν_1 and ν_2 and $\Delta_{12} = \nu_1 - \omega_{12}$, $\Delta_{23} = \nu_2 - \omega_{23}$ are the detunings. We assume the case of exact two-photon resonance, which means that

$$\Delta_{12} = -\Delta_{23} = \Delta. \tag{50}$$

Under these assumptions the Hamiltonian becomes

$$\hat{H} = - \begin{pmatrix} 0 & \frac{1}{2}\Omega_{12} & 0 \\ \frac{1}{2}\Omega_{12} & \Delta & \frac{1}{2}\Omega_{23} \\ 0 & \frac{1}{2}\Omega_{23} & 0 \end{pmatrix}. \quad (51)$$

Here $\Omega_{12} = \underline{d}_{12} \cdot \underline{\mathcal{E}}_1$ and $\Omega_{23} = \underline{d}_{23} \cdot \underline{\mathcal{E}}_2$ are the Rabi frequencies, \underline{d}_{jk} is the atomic dipole moment between levels j and k and $\underline{\mathcal{E}}_1$ and $\underline{\mathcal{E}}_2$ are the vector amplitudes of electric fields of the lasers. We assume that the Rabi frequencies Ω_{12}, Ω_{23} have a specific form given by

$$\Omega_{12}(t) = 2a\Omega_0(t) \quad (52)$$

$$\Omega_{23}(t) = 2b\Omega_0(t), \quad (53)$$

where a and b are non-negative real numbers. This means that Ω_{12} and Ω_{23} have the same time dependence but possibly different amplitudes. In the present case equation (43) gives

$$\left(\frac{d\underline{\lambda}}{dt} \right)^T = V\underline{\lambda}^T, \quad (54)$$

where

$$V = \begin{pmatrix} 0 & 0 & 0 & -\Delta & -b\Omega_0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -b\Omega_0 & 0 & a\Omega_0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a\Omega_0 & \Delta & 0 & 0 \\ \Delta & b\Omega_0 & 0 & 0 & 0 & 0 & 2a\Omega_0 & 0 \\ b\Omega_0 & 0 & -a\Omega_0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -a\Omega_0 & -\Delta & 0 & 0 & 0 & -b\Omega_0 & \sqrt{3}b\Omega_0 \\ 0 & 0 & 0 & -2a\Omega_0 & 0 & b\Omega_0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\sqrt{3}b\Omega_0 & 0 & 0 \end{pmatrix} \quad (55)$$

and T denotes transpose. In order to simplify (54) we define a new basis $\{\hat{\lambda}'_1, \dots, \hat{\lambda}'_8\}$ through the equation

$$\hat{\underline{\lambda}}'^T = B\hat{\underline{\lambda}}^T. \quad (56)$$

Here $\hat{\underline{\lambda}} = (\hat{\lambda}_1, \dots, \hat{\lambda}_8)$ and $\hat{\underline{\lambda}}' = (\hat{\lambda}'_1, \dots, \hat{\lambda}'_8)$ are vectors formed from the generators of $SU(3)$ and the basis change is given by the time independent orthogonal matrix

$$B = \frac{1}{\sqrt{a^2 + b^2}} \begin{pmatrix} a & 0 & b & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 0 & -b & 0 & 0 \\ 0 & \frac{ab}{\sqrt{a^2 + b^2}} & 0 & 0 & 0 & 0 & \frac{2a^2 + b^2}{2\sqrt{a^2 + b^2}} & -\frac{\sqrt{3}b^2}{2\sqrt{a^2 + b^2}} \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ b & 0 & -a & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -b & 0 & -a & 0 & 0 \\ 0 & \frac{-a^2 + b^2}{\sqrt{a^2 + b^2}} & 0 & 0 & 0 & 0 & \frac{ab}{\sqrt{a^2 + b^2}} & \frac{\sqrt{3}ab}{\sqrt{a^2 + b^2}} \\ 0 & -\frac{\sqrt{3}ab}{\sqrt{a^2 + b^2}} & 0 & 0 & 0 & 0 & \frac{\sqrt{3}b^2}{2\sqrt{a^2 + b^2}} & \frac{-2a^2 + b^2}{2\sqrt{a^2 + b^2}} \end{pmatrix} \quad (57)$$

In the new basis the time-evolution can be solved from

$$\frac{d}{dt}\underline{\lambda}'^T = V'\underline{\lambda}'^T, \quad (58)$$

where V' is a block-diagonal matrix given by

$$V' = BV B^T = \begin{pmatrix} V'_3 & & \\ & V'_4 & \\ & & V'_1 \end{pmatrix} \quad (59)$$

and

$$V'_3 = \begin{pmatrix} 0 & -\Delta & 0 \\ \Delta & 0 & 2\epsilon \\ 0 & -2\epsilon & 0 \end{pmatrix}, \quad V'_4 = \begin{pmatrix} 0 & -\epsilon & 0 & 0 \\ \epsilon & 0 & \Delta & 0 \\ 0 & -\Delta & 0 & -\epsilon \\ 0 & 0 & \epsilon & 0 \end{pmatrix}, \quad V'_1 = 0 \quad (60)$$

with

$$\epsilon = \Omega_0 \sqrt{a^2 + b^2}. \quad (61)$$

This result means that the time-evolution of the system can be analyzed in terms of three separate vectors:

$$\underline{\Lambda}_3 = (\lambda'_1, \lambda'_2, \lambda'_3), \quad \underline{\Lambda}_4 = (\lambda'_4, \lambda'_5, \lambda'_6, \lambda'_7), \quad \underline{\Lambda}_1 = (\lambda'_8), \quad (62)$$

Because of the antisymmetry of the V' -matrices, the lengths of these vectors are conserved

$$|\underline{\Lambda}_3| = \text{const.}, \quad |\underline{\Lambda}_4| = \text{const.}, \quad |\underline{\Lambda}_1| = \text{const.} \quad (63)$$

These are not independent quantities as they are tied together by the normalization condition $|\underline{\Lambda}_3|^2 + |\underline{\Lambda}_4|^2 + |\underline{\Lambda}_1|^2 = |\underline{\lambda}'|^2 = \text{const.}$ Therefore, in the presence of two monochromatic lasers and under two-photon resonance, there are two conserved quantities in addition to the one arising from the conservation of $|\lambda'|$. Due to unitary time-evolution $\underline{\lambda}'(t) = \underline{\Lambda}_3(t) \oplus \underline{\Lambda}_4(t) \oplus \underline{\Lambda}_1(t)$ assumes only values which produce a positive density matrix $\rho(t)$. Using (57) the conserved quantities (63) can be expressed in terms of the components of the original Bloch vector $\underline{\lambda}$. For example, the time-independence of $|\Lambda_1|$ means that

$$\left(2\sqrt{3}ab\lambda_2(t) + \sqrt{3}b^2\lambda_7(t) - (2a^2 - b^2)\lambda_8(t) \right)^2 = \text{const} \times (a^2 + b^2)^2, \quad (64)$$

where the value of the constant is determined by the initial values of λ_2, λ_7 , and λ_8 . In (7, 61) it has been shown that similar approach allows to identify two constants of motion in a three-level system under the assumption that the Rabi frequencies are sinusoidally modulated, with a phase difference $\pi/2$ between them. In this case the matrix determining the time-evolution is not block diagonal but enables nevertheless the time-evolution to be solved.

This approach has been extended to systems with more than three levels (9). If the Hamiltonian has a certain form, obtained by defining a counterpart of the Hamiltonian (51) in the n level case, n conserved quantities can be identified.

2.5. The Bloch vector of two-qubit system

We now study the Bloch vector description of a system consisting of two qubits, denoted by A and B . The Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B = \mathbb{C}^2 \otimes \mathbb{C}^2$ is four dimensional and the density matrices can be expressed using the generalized 4×4 Gell-Mann matrices (28). However, instead of using this basis, it is often advantageous to define the basis in terms of the basis elements of the Lie algebra of $SU(2) \otimes SU(2)$. This approach has been used in many articles,

see, for example, (4, 10–18). The latter choice for the basis allows to examine the entanglement of two-qubit systems in a more natural way than the generalized Gell-Mann matrix basis. We choose the basis $\{\hat{\lambda}_1, \hat{\lambda}_2, \dots, \hat{\lambda}_{15}\}$ of the Lie algebra of $SU(2) \otimes SU(2)$ as

$$\hat{\lambda}_i = \frac{1}{\sqrt{2}} \sigma_i \otimes I_2, \quad i = 1, 2, 3 \quad (65)$$

$$\hat{\lambda}_i = \frac{1}{\sqrt{2}} I_2 \otimes \sigma_{i-3} \quad i = 4, 5, 6 \quad (66)$$

$$\hat{\lambda}_i = \frac{1}{\sqrt{2}} \sigma_1 \otimes \sigma_{i-6} \quad i = 7, 8, 9 \quad (67)$$

$$\hat{\lambda}_i = \frac{1}{\sqrt{2}} \sigma_2 \otimes \sigma_{i-9} \quad i = 10, 11, 12 \quad (68)$$

$$\hat{\lambda}_i = \frac{1}{\sqrt{2}} \sigma_3 \otimes \sigma_{i-12} \quad i = 13, 14, 15. \quad (69)$$

This forms an orthogonal basis with respect to trace with the normalization given by

$$\text{Tr}(\hat{\lambda}_i \hat{\lambda}_j) = 2 \delta_{ij}. \quad (70)$$

The totally symmetric structure constants are

$$\begin{aligned} g_{147} = g_{158} = g_{169} = g_{24(10)} = g_{25(11)} = g_{26(12)} = g_{34(13)} = g_{35(14)} = g_{36(15)} \\ = -g_{7(11)(15)} = g_{7(12)(14)} = g_{8(10)(15)} = -g_{8(12)(13)} = -g_{9(10)(14)} = g_{9(11)(13)} = \frac{1}{\sqrt{2}}. \end{aligned} \quad (71)$$

These are needed in the calculation of the coefficients of the characteristic polynomial. An arbitrary two-qubit state can be expressed as

$$\rho = \frac{1}{4} I_4 + \frac{1}{2} \sum_{i=1}^{15} \lambda_i \hat{\lambda}_i \quad (72)$$

$$= \frac{1}{2\sqrt{2}} \left(\frac{1}{\sqrt{2}} I_4 + \sum_{i=1}^3 \lambda_i \sigma_i \otimes I_2 + \sum_{i=1}^3 \lambda_{i+3} I_2 \otimes \sigma_i + \sum_{i=1}^3 \sum_{j=1}^3 \lambda_{j+3i+3} \sigma_i \otimes \sigma_j \right), \quad (73)$$

where $\underline{\lambda}$ is assumed to be such that ρ is positive. The reduced single-particle density matrices determined by this state are

$$\rho_A = \text{Tr}_B(\rho) = \frac{1}{2} I_2 + \frac{1}{\sqrt{2}} \sum_{i=1}^3 \lambda_i \sigma_i, \quad \rho_B = \text{Tr}_A(\rho) = \frac{1}{2} I_2 + \frac{1}{\sqrt{2}} \sum_{i=1}^3 \lambda_{i+3} \sigma_i \quad (74)$$

Here Tr_A denotes trace over subsystem A , Tr_B is defined similarly. The components of the Bloch vectors of the reduced states are uniquely obtained from the components of the Bloch vector of ρ . The inverse does not hold; any information regarding the $\lambda_7, \lambda_8, \dots, \lambda_{15}$ components of the Bloch vector is missing from the reduced states ρ_A and ρ_B . The knowledge of the Bloch vectors of ρ_A and ρ_B does not allow to construct a *unique* two-qubit Bloch vector which gives rise to ρ_A and ρ_B .

As an example of the use of the parametrization we consider the Werner state for two qubits

$$\rho_W(x) = \frac{1-x}{4} I_4 + xS, \quad (75)$$

where x is a real parameter and S is

$$S = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (76)$$

We first determine the range of the parameter x which ensures positivity of $\rho_W(x)$, making sure that $\rho_W(x)$ indeed is a density operator. After this we study the separability of the Werner state $W(x)$. We may write $W(x)$ as

$$\begin{aligned} W(x) &= \frac{1}{4}I_4 - \frac{x}{4}(\sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3) \\ &= \frac{1}{4} \begin{pmatrix} 1-x & 0 & 0 & 0 \\ 0 & 1+x & -2x & 0 \\ 0 & -2x & 1+x & 0 \\ 0 & 0 & 0 & 1-x \end{pmatrix}. \end{aligned} \quad (77)$$

The only non-zero components of the Bloch vector are $\lambda_7 = \lambda_{11} = \lambda_{15} = -x/\sqrt{2}$. A straightforward calculation gives the coefficients of the characteristic polynomial (36)

$$1!a_1 = 1 \quad (78)$$

$$2!a_2 = \frac{3}{4}(1-x^2) \quad (79)$$

$$3!a_3 = \frac{3}{8}(1-3x^2+2x^3) \quad (80)$$

$$4!a_4 = \frac{3}{32}(1-6x^2+8x^3-3x^4) \quad (81)$$

These are all non-negative when $-1/3 \leq x \leq 1$, which is therefore the range of x corresponding to physical states. Usually, however, the range of x is taken to be $[0, 1]$. We now examine the separability of $W(x)$. The density matrix ρ of a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$ is called *separable* when it can be written as a probabilistic mixture of tensor product states

$$\rho = \sum_i p_i \rho_A^i \otimes \rho_B^i, \quad p_i \geq 0, \quad \sum_i p_i = 1. \quad (82)$$

If a state is not separable it is *entangled*. Detecting separability is in general a very complicated problem, but in some special cases it can be done easily. A simple way to test the separability of a two-qubit system is to use the Peres-Horodecki, or positive partial transposition, criterion (62, 63). It provides a necessary and sufficient condition for separability for 2×2 and 2×3 dimensional systems. According to this criterion, a state ρ is separable if the operator obtained by transposing the density operator of the subsystem A or B is a positive operator. When the state of the second subsystem is transposed, (73) becomes

$$\rho^{\text{pt}} = \frac{1}{2\sqrt{2}} \left(\frac{1}{\sqrt{2}}I_4 + \sum_{i=1}^3 \lambda_i \sigma_i \otimes I_2 + \sum_{i=1}^3 \lambda_{i+3} I_2 \otimes \sigma_i^T + \sum_{i=1}^3 \sum_{j=1}^3 \lambda_{j+3i+3} \sigma_i \otimes \sigma_j^T \right) \quad (83)$$

$$= \frac{1}{2\sqrt{2}} \left(\frac{1}{\sqrt{2}}I_4 + \sum_{i=1}^3 \lambda_i^{\text{pt}} \sigma_i \otimes I_2 + \sum_{i=1}^3 \lambda_{i+3}^{\text{pt}} I_2 \otimes \sigma_i + \sum_{i=1}^3 \sum_{j=1}^3 \lambda_{j+3i+3}^{\text{pt}} \sigma_i \otimes \sigma_j \right), \quad (84)$$

where $\lambda_5^{\text{pt}} = -\lambda_5$, $\lambda_8^{\text{pt}} = -\lambda_8$, $\lambda_{11}^{\text{pt}} = -\lambda_{11}$, $\lambda_{14}^{\text{pt}} = -\lambda_{14}$ and $\lambda_i^{\text{pt}} = \lambda_i$ for the rest of the components. When partial transpose is applied to the Werner state we get

$$\begin{aligned} W_{\text{pt}}(x) &= \frac{1}{4}I_4 - \frac{x}{4}(\sigma_1 \otimes \sigma_1 - \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3) \\ &= \frac{1}{4} \begin{pmatrix} 1-x & 0 & 0 & -2x \\ 0 & 1+x & 0 & 0 \\ 0 & 0 & 1+x & 0 \\ -2x & 0 & 0 & 1-x \end{pmatrix}. \end{aligned} \quad (85)$$

The calculation of the coefficients a_i^{pt} of the characteristic polynomial of $W_{\text{pt}}(x)$ shows that a_1^{pt} and a_2^{pt} are the same than for $W(x)$ and

$$3!a_3^{\text{pt}} = \frac{3}{8}(1 - 3x^2 - 2x^3) \quad (86)$$

$$4!a_4^{\text{pt}} = \frac{3}{32}(1 - 6x^2 - 8x^3 - 3x^4). \quad (87)$$

These differ from a_3 and a_4 by the sign of the x^3 -term. These coefficients are non-negative when $-1 \leq x \leq 1/3$. Therefore the Werner state $W(x)$ is separable when $-1/3 \leq x \leq 1/3$ and entangled when $1/3 < x \leq 1$. Because $W(x)$ is obtained by partially transposing $W_{\text{pt}}(x)$, the state $W_{\text{pt}}(x)$ is separable when $-1/3 \leq x \leq 1/3$ and entangled when $-1 \leq x < -1/3$.

2.6. The polarization operator basis

Our definition of the Bloch vector with respect to the generalized Gell-Mann matrices is not the only possible. Although changing the basis will change the Bloch vector representation of the states, it does not affect the structure of the set of density matrices in general. One possible way to choose the basis is to use the polarization operators, also known as spherical tensor operators. The concept of a polarization operator appears in the quantum mechanical theory of angular momentum and is thoroughly discussed in the literature, see, for example, (64, 65). When the angular symmetries of the system are important it is convenient to expand ρ using the polarization operators. Many examples of such systems can be found in (21). We will describe the polarization operators only briefly. In the following discussion we define the basis and characterize some of the properties of the set of Bloch vectors corresponding to physical states. This subsection is based on (19, 20).

The polarization operators pertaining to an n -level system are defined as

$$T_{LM} = \sqrt{\frac{2L+1}{2s+1}} \sum_{k,l=1}^n C_{sm_l, LM}^{sm_k} |k\rangle \langle l|, \quad (88)$$

where the indices have the properties

$$\begin{aligned} s &= \frac{n-1}{2}, \\ L &= 0, 1, \dots, 2s, \\ M &= -L, -L+1, \dots, L-1, L, \\ m_1 &= s, \quad m_2 = s-1, \dots, m_n = -s. \end{aligned} \quad (89)$$

The coefficients $C_{sm_l, LM}^{sm_k}$ are identified with the usual Clebsch–Gordan coefficients $C_{j_1 m_1, j_2 m_2}^{j m}$ of

the theory angular momentum. For $L = M = 0$ the polarization operator is proportional to the identity matrix

$$T_{00} = \frac{1}{\sqrt{n}} I_n. \quad (90)$$

All other polarization operators are traceless, but they are *not* Hermitian in general. Due to the symmetry properties of the Clebsch–Gordan coefficients they satisfy the orthogonality relation

$$\text{Tr}(T_{L_1 M_1}^\dagger T_{L_2 M_2}) = \delta_{L_1 L_2} \delta_{M_1 M_2} \quad (91)$$

and they have the property

$$T_{LM}^\dagger = (-1)^M T_{L-M}. \quad (92)$$

The former equation ensures that the polarization operators form an orthonormal basis. Any density matrix can be written using this basis as

$$\rho = \frac{1}{n} I_n + \sum_{L=1}^{2s} \sum_{M=-L}^L \lambda_{LM}^{\text{po}} T_{LM} = \frac{1}{n} I_n + \underline{\lambda}^{\text{po}} \cdot \underline{T} \quad (93)$$

with the Bloch vector in the polarization operator basis given by $\underline{\lambda}^{\text{po}} = (\lambda_{1-1}^{\text{po}}, \lambda_{10}^{\text{po}}, \lambda_{11}^{\text{po}}, \lambda_{2-2}^{\text{po}}, \lambda_{2-1}^{\text{po}}, \lambda_{20}^{\text{po}}, \dots, \lambda_{(n-1)(n-1)}^{\text{po}})$, where the components are ordered and given by $\lambda_{LM}^{\text{po}} = \text{Tr}(T_{LM}^\dagger \rho)$. In general, the components λ_{LM}^{po} are complex since the polarization operators are not Hermitian. The hermiticity of the density matrix, $\rho = \rho^*$, forces the components of the Bloch vector to fulfill the condition

$$\lambda_{LM}^{\text{po}} = (-1)^M \bar{\lambda}_{L-M}^{\text{po}} \quad (94)$$

In particular, the components λ_{L0}^{po} are real. In order for ρ to describe a physical state it also has to be positive. As in the case of the Gell-Mann matrix basis, the positivity of ρ can be checked using (29) and (32). The coefficients a_j of the characteristic polynomial (29) are related to the trace invariants through the equation

$$ja_j = \sum_{m=1}^j (-1)^{m-1} a_{j-m} \text{Tr}(\rho^m). \quad (95)$$

General expression for the trace invariants can be calculated to be

$$\begin{aligned} \text{Tr}(\rho^k) &= \frac{1}{n^{k-1}} + \frac{k(k-1)}{2n^{k-2}} |\underline{\lambda}^{\text{po}}|^2 + \sum_{m=3}^k \binom{k}{m} \frac{\text{Tr}[(\underline{\lambda}^{\text{po}} \cdot \underline{T})^m]}{n^{k-m}}, \\ \text{Tr}[(\underline{\lambda}^{\text{po}} \cdot \underline{T})^m] &= \sum_{L_1=1}^{n-1} \sum_{M_1=-L_1}^{L_1} \cdots \sum_{L_m=1}^{n-1} \sum_{M_m=-L_m}^{L_m} \lambda_{L_1 M_1}^{\text{po}} \cdots \lambda_{L_m M_m}^{\text{po}} \text{Tr}(T_{L_1 M_1} \cdots T_{L_m M_m}). \end{aligned} \quad (96)$$

The traces can be calculated using the equations presented in (65). Combining the results we find that the coefficients of the characteristic polynomial are

$$ja_j = a_{j-1} + \sum_{k=2}^j (-1)^{k-1} a_{j-k} \left[\frac{1}{n^{k-1}} + \sum_{m=2}^k \binom{k}{m} \frac{\text{Tr}[(\underline{\lambda}^{\text{po}} \cdot \underline{T})^m]}{n^{k-m}} \right]. \quad (97)$$

The first three coefficients are $a_0 = a_1 = 1$ and

$$2a_2 = 1 - \frac{1}{n} - |\underline{\lambda}^{\text{po}}|^2. \quad (98)$$

Therefore a necessary condition for ρ to be a positive operator is that Bloch vectors lie within a hypersphere of radius $|\underline{\lambda}^{\text{po}}| \leq \sqrt{(n-1)/n}$. In the case of a two-level system ($n = 2$) the density matrix becomes

$$\rho = \frac{1}{2}I_2 + (\alpha + i\beta)T_{11} - (\alpha - i\beta)T_{1-1} + \gamma T_{00}, \quad (99)$$

where α, β, γ are real and we have defined $\lambda_{11}^{\text{po}} = \alpha + i\beta$, $\lambda_{00}^{\text{po}} = \gamma$ and used (94). The set of physical states is now given by $Q_2 = \{(\alpha, \beta, \gamma) \in \mathbb{R}^3 \mid 2(\alpha^2 + \beta^2) + \gamma^2 \leq 1/2\}$. The surface of this set corresponds to pure states and is a prolate spheroid.

As in the case of the Bloch vector given in the generalized Gell-Mann basis, for $n \geq 3$ the structure of the set of physical states becomes very complicated (19). Nevertheless, pure states are on the surface, mixed ones lie within the volume and the maximally mixed state corresponds to $|\underline{\lambda}^{\text{po}}| = 0$.

3. The coset parametrization

This section presents a short summary of the article (28). If $D = D_n(\lambda_1, \dots, \lambda_n)$ is the diagonal matrix of eigenvalues in the spectral representation (9) of a density matrix ρ , we denote by D' the commutant of D in $U(n)$, i.e., the set of all matrices $U \in U(n)$ such that $UD = DU$. Now, if (9) holds for some $U \in U(n)$ and V is some other unitary matrix such that $VU^{-1} \in D'$ then one has

$$\rho = U^*DU = V^*DV, \quad VU^{-1} \in D', \quad (100)$$

and conversely.

In the case of nondegenerate spectrum the commutant D' is easily determined:

$$D' = T^n = U(1) \otimes \dots \otimes U(1), \quad n \text{ factors}, \quad (101)$$

and thus one can say

$$\rho = \Omega^*D\Omega, \quad \Omega \in U(n)/T^n. \quad (102)$$

According to the book (38) elements $U \in U(n)$ can be factored in the following way:

$$U = \Omega_n \Omega_{n-1} \dots \Omega_2 \Omega_1 \quad (103)$$

with $\Omega_1 \in T^n$ and

$$\Omega_k \in \frac{U(k) \otimes T^{n-k}}{U(k-1) \otimes T^{n-k+1}}, \quad k = 2, \dots, n. \quad (104)$$

Typical coset representatives Ω_k are of the form

$$\left(\begin{array}{c|c} SU(k)/U(k-1) & \mathbb{O} \\ \hline \mathbb{O}^T & I_{n-k} \end{array} \right) \quad (105)$$

where \mathbb{O} is the $k \times (n - k)$ zero matrix and \mathbb{O}^T its transpose while I_{n-k} denotes the $n - k$ dimensional unit matrix.

After a brief sketch of the general case the article (28) proceeds to discuss in some detail the cases $n = 2$ and $n = 3$ (and the Bures metric and the $n = 2$ state space). A more systematic approach and an explicit realization of the factorization (103) is given in the following section. Therefore no further details are presented here.

4. The Jarlskog parametrization

Like the coset parametrization also the Jarlskog parametrization starts from the spectral representation (9) of a density matrix. Accordingly, we begin with a concrete version of the factorization of a unitary matrix $U_n \in SU(n)$ in terms of certain basic unitary matrices as in (103) following (24). Since this factorization is based on the use of canonical coordinates of second kind in the Lie group $SU(n)$, a more accurate name for the parametrization would be the “canonical coordinate parametrization”. Some preliminary investigations into this problem have been given in the article (40). After having defined the Jarlskog parametrization of unitary matrices, we show how it can be used to parametrize density matrices. As an application of this parametrization we construct a general density matrix of a two-level system. We also show that the Jarlskog parametrization can be straightforwardly extended to composite systems and illustrate this by constructing some two-qubit states.

4.1. Jarlskog’s recursive parametrization of unitary matrices

Recall that the Lie group $U(n)$ is connected but not simply connected and that every $U_n \in U(n)$ has a determinant of absolute value 1. It follows that every $U_n \in U(n)$ has a determinant $\det U_n = e^{i\alpha}$ and thus can be written as

$$U_n = D_n(e^{i\alpha}, 1, \dots, 1)U'_n, \quad \alpha \in \mathbb{R}, \quad U'_n \in SU(n)$$

where $SU(n)$ denotes the Lie group of unitary matrices of determinant 1. Obviously, the diagonal matrices $D_n(e^{i\alpha}, 1, \dots, 1)$ and $D_n(\lambda_1, \dots, \lambda_n)$ commute and hence in (9) we can restrict ourselves to unitary matrices in $SU(n)$, i.e., $\rho_n \in \mathcal{D}_n$ if, and only if,

$$\rho_n = U_n^* D_n(\lambda_1, \dots, \lambda_n) U_n, \quad U_n \in SU(n). \quad (106)$$

where the eigenvalues λ_j satisfy (7) and (8). This reduces our problem to that of finding a parametrization of unitary matrices of determinant 1.

In order to provide the necessary background for this parametrization of unitary matrices and the important recursion formula we follow Fujii (66) to explain the origin of the basic building blocks of this parametrization. He observed that the Jarlskog parametrization of unitary matrices is obtained by using canonical coordinates of the second kind for the Lie group $SU(n)$ (see, for instance, (67)).

Recall that $SU(n)$ is the (simply) connected component of the unit element of $U(n)$ and thus is the image of its Lie algebra $su(n)$ under the exponential map. The Lie algebra $su(n)$ consists

of all skew-adjoint $n \times n$ matrices X . Such matrices have the form

$$X = \begin{pmatrix} i\alpha_1 & z_{12} & z_{13} & \cdots & z_{1,n-1} & z_{1n} \\ -\bar{z}_{12} & i\alpha_2 & z_{23} & \cdots & z_{2,n-1} & z_{2n} \\ -\bar{z}_{13} & -\bar{z}_{23} & i\alpha_3 & \cdots & z_{3,n-1} & z_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ -\bar{z}_{1,n-1} & -\bar{z}_{2,n-1} & \bar{z}_{3,n-1} & \cdots & i\alpha_{n-1} & z_{n-1,n} \\ -\bar{z}_{1,n} & -\bar{z}_{2,n} & -\bar{z}_{3,n} & \cdots & -\bar{z}_{n-1,n} & i\alpha_n \end{pmatrix} \quad (107)$$

where the α_j 's are real numbers and the z_{jk} are complex numbers which can be chosen independently. Such a matrix has the natural decomposition

$$X = X_1 + X_2 + \cdots + X_j + \cdots + X_n \quad (108)$$

where X_1 is the diagonal matrix with the diagonal entries $i\alpha_1, \dots, i\alpha_n$:

$$X_1 = D_n(i\alpha_1, \dots, i\alpha_n) \quad (109)$$

and where for $j = 2, \dots, n$ the matrix X_j is the matrix which has in column j the column vector

$$|z_j\rangle = \begin{pmatrix} z_{1j} \\ z_{2j} \\ \vdots \\ z_{j-1,j} \end{pmatrix} \in \mathbb{C}^{j-1} \quad (110)$$

and in row j the row vector

$$-\langle z_j| = (-\bar{z}_{1j}, -\bar{z}_{2j}, \dots, -\bar{z}_{j-1,j}) \quad (111)$$

as entries. All other entries of X_j are zero.

The canonical coordinates of the second kind for $SU(n)$ are given by

$$su(n) \ni X = X_1 + X_2 + \cdots + X_j + \cdots + X_n \longrightarrow e^{X_1} e^{X_2} \cdots e^{X_j} \cdots e^{X_n} \in SU(n). \quad (112)$$

The exponential e^{X_1} is easily calculated:

$$A_{n,1} = e^{X_1} = A_{n,1}(\alpha_1, \dots, \alpha_n) = D_n(e^{i\alpha_1}, \dots, e^{i\alpha_n}), \quad \alpha_j \in \mathbb{R}. \quad (113)$$

For $j = 2, \dots, n-1$ we write

$$X_j = \begin{pmatrix} K_j & \mathbb{O} \\ \mathbb{O} & \mathbb{O}_{n-j} \end{pmatrix}, \quad K_j = \begin{pmatrix} \mathbb{O}_{j-1} & |z_j\rangle \\ -\langle z_j| & \mathbb{O} \end{pmatrix}, \quad (114)$$

where \mathbb{O}_k denotes the $k \times k$ zero matrix and \mathbb{O} indicates that the remaining entries of the matrix are zero. Naturally $X_n = K_n$. Thus we get

$$e^{X_j} = \begin{pmatrix} e^{K_j} & \mathbb{O} \\ \mathbb{O} & I_{n-j} \end{pmatrix}, \quad j = 2, \dots, n-1, \quad e^{X_n} = e^{K_n} \quad (115)$$

where I_k denotes the $k \times k$ unit matrix. Using

$$K_j^2 = - \begin{pmatrix} |z_j\rangle\langle z_j| & 0 \\ \mathbb{O} & \langle z_j|z_j\rangle \end{pmatrix}, \quad K_j^3 = -\langle z_j|z_j\rangle K_j$$

one can calculate the exponentials and finds for $j = 2, \dots, n$, $|z_j| = \sqrt{\langle z_j|z_j\rangle}$,

$$e^{K_j} = I_j + (1 - \cos |z_j|) \frac{1}{|z_j|^2} K_j^2 + \sin |z_j| \frac{1}{|z_j|} K_j. \quad (116)$$

If one introduces the unit vector $|\tilde{z}_j\rangle = \frac{1}{|z_j|}|z_j\rangle \in \mathbb{C}^{j-1}$ one can rewrite this exponential as

$$e^{K_j} = I_j - (1 - \cos |z_j|) \begin{pmatrix} |\tilde{z}_j\rangle\langle\tilde{z}_j| & 0 \\ \mathbb{O} & 1 \end{pmatrix} + \sin |z_j| \begin{pmatrix} \mathbb{O}_{j-1} & |\tilde{z}_j\rangle \\ -\langle\tilde{z}_j| & 0 \end{pmatrix}. \quad (117)$$

The right hand side of (117) is a unitary matrix $V_{n,j}$ which is often written as

$$V_{n,j} = \begin{pmatrix} I_{j-1} - (1 - c_j)|\tilde{z}_j\rangle\langle\tilde{z}_j| & s_j|\tilde{z}_j\rangle \\ -s_j\langle\tilde{z}_j| & c_j \end{pmatrix}, \quad c_j = \cos |z_j|, \quad s_j = \sin |z_j|. \quad (118)$$

Since the adjoint (and the inverse) of the matrix e^{K_j} is e^{-K_j} , the adjoint and the inverse of the matrix $V_{n,j}$ is given by (118) with \tilde{z}_j replaced by $-\tilde{z}_j$.

The Jarlskog matrices $A_{n,j} = e^{X_j}$, $j = 1, \dots, n$ (see (22, 24)) thus are of the form

$$A_{n,j} = \begin{pmatrix} V_{n,j} & \mathbb{O} \\ \mathbb{O} & I_{n-j} \end{pmatrix}, \quad j = 2, \dots, n-1, \quad A_{n,n} = V_{n,n}. \quad (119)$$

A generic element $U_n \in SU(n)$ therefore has the factorization

$$U_n = e^{X_1} e^{X_2} \dots e^{X_n} = A_{n,1} A_{n,2} \dots A_{n,n} \quad (120)$$

or equivalently

$$U_n = e^{X_n} e^{X_{n-1}} \dots e^{X_1} = A_{n,n} A_{n,n-1} \dots A_{n,1}. \quad (121)$$

Observe that by construction the Jarlskog matrix $A_{n,j}$ is defined in terms of the following set of parameters

$$\theta_j \geq 0, \quad z_j \in S(\mathbb{C}^{j-1})$$

where we changed notation: θ_j for $|z_j|$ and z_j for \tilde{z}_j , and where $S(\mathbb{C}^{j-1})$ denotes the unit sphere in \mathbb{C}^{j-1} . We indicate this by writing $A_{n,j} = A_{n,j}(\theta_j, z_j)$. The special structure of the matrix $A_{n,j}$ and the properties of the trigonometric functions imply that on the parameter set

$$P_{n,j} = \{(\theta_j, z_j) : 0 \leq \theta_j \leq \pi/2, z_j \in S(\mathbb{C}^{j-1})\} \quad (122)$$

the mapping $(\theta_j, z_j) \longrightarrow A_{n,j}$ is injective, i.e., if $(\theta_j, z_j), (\theta'_j, z'_j) \in P_{n,j}$ and $A_{n,j}(\theta_j, z_j) = A_{n,j}(\theta'_j, z'_j)$ then $\theta_j = \theta'_j$ and $z_j = z'_j$.

According to (107) or (120), (121) and (122) this factorization describes a generic element $U_n \in SU(n)$ in terms of n^2 real parameters.

Notice that the matrices $V_{n,j}$ do not depend explicitly on the dimension n and that we can write, for $j = 2, \dots, n-1$,

$$A_{n,j} = \begin{pmatrix} \tilde{V}_{n,j} & \mathbb{O} \\ \mathbb{O} & 1 \end{pmatrix}, \quad \tilde{V}_{n,j} = \begin{pmatrix} V_{n,j} & \mathbb{O} \\ \mathbb{O} & I_{n-j-1} \end{pmatrix}. \quad (123)$$

It follows that

$$A_{n,1} \cdots A_{n,n-1} = \begin{pmatrix} \tilde{V}_{n,1} \cdots \tilde{V}_{n,n-1} & \mathbb{O} \\ \mathbb{O} & 1 \end{pmatrix}. \quad (124)$$

The analysis presented above shows that $\tilde{V}_{n,1} \cdots \tilde{V}_{n,n-1}$, up to a factor in T^{n-1} , gives the generic factorization of $(n-1) \times (n-1)$ special unitary matrices and hence, from (121), we get the important recursion relation

$$U_n = \begin{pmatrix} U_{n-1} & \mathbb{O} \\ \mathbb{O} & 1 \end{pmatrix} A_{n,n} = \begin{pmatrix} U_{n-1} & \mathbb{O} \\ \mathbb{O} & 1 \end{pmatrix} \begin{pmatrix} I_{n-1} - (1-c_n)|z_n\rangle\langle z_n| & s_n|z_n\rangle \\ -s_n\langle z_n| & c_n \end{pmatrix} \quad (125)$$

Next we address the question of injectivity of the Jarlskog parametrization of $U_n \in SU(n)$ modulo elements in T^n , i.e., the parametrization (120) without the factor $A_{n,1} \in T^n$. Then this parametrization uses the parameter set

$$P_n = \{(\theta_j, z_j) : (\theta_j, z_j) \in P_{n,j}, j = 2, \dots, n\} \quad (126)$$

where we have taken (120) and (122) into account. In order to prove injectivity of the map

$$(\theta_2, z_2; \theta_3, z_3; \dots; \theta_n, z_n) \longrightarrow U_n = A_{n,2}(\theta_2, z_2)A_{n,3}(\theta_3, z_3) \cdots A_{n,n}(\theta_n, z_n), \quad (127)$$

where $(\theta_2, z_2; \theta_3, z_3; \dots; \theta_n, z_n) \in P_n$, we proceed by induction with respect to the order n . Since $(\theta_j, z_j) \longrightarrow A_{n,j}$ is injective on $P_{n,j}$, the map (127) is injective for $n = 2$. Now assume that for some $n > 2$ this map is injective for the orders $k \leq n-1$. We now show that the map (127) then is injective for the order $k = n$.

Suppose that for $U_n, U'_n \in SU(n)$ we have $U'_n = U_n$ where $U'_n = U_n(\theta'_2, z'_2; \theta'_3, z'_3; \dots; \theta'_n, z'_n)$. In the recursion formula (125) for U_n we abbreviate $I_{n-1} - (1-c_n)|z_n\rangle\langle z_n|$ with B_{n-1} and similarly for U'_n and B'_{n-1} . If we calculate the matrix product in the recursion relation, the identity $U'_n = U_n$ reads

$$\begin{pmatrix} U'_{n-1}B'_{n-1} & s'_n U'_{n-1}|z'_n\rangle \\ -s'_n \langle z'_n| & c'_n \end{pmatrix} = \begin{pmatrix} U_{n-1}B_{n-1} & s_n U_{n-1}|z_n\rangle \\ -s_n \langle z_n| & c_n \end{pmatrix} \quad (128)$$

where we used the abbreviations $s'_n = \sin \theta'_n$ and $c'_n = \cos \theta'_n$. Thus $c'_n = c_n$; since $\theta_n, \theta'_n \in [0, \pi/2]$ we conclude $\theta'_n = \theta_n$ and therefore $s'_n = s_n$. The identity $-s'_n \langle z'_n| = -s_n \langle z_n|$ now implies $\langle z'_n| = \langle z_n|$ and $|z'_n\rangle = |z_n\rangle$. Next we use the identity $s'_n U'_{n-1}|z'_n\rangle = s_n U_{n-1}|z_n\rangle$ to conclude $U'_{n-1}|z'_n\rangle = U_{n-1}|z_n\rangle = U_{n-1}|z_n\rangle$. Finally we use the identity $U'_{n-1}B'_{n-1} = U_{n-1}B_{n-1}$ to get

$$U'_{n-1} - (1-c'_n)U'_{n-1}|z'_n\rangle\langle z'_n| = U_{n-1} - (1-c_n)U_{n-1}|z_n\rangle\langle z_n|$$

and from the identities established above we find $U'_{n-1} = U_{n-1}$. The induction hypothesis implies $(\theta'_j, z'_j) = (\theta_j, z_j)$ for $j = 2, \dots, n-1$, and we conclude.

4.2. Jarlskog parametrization

Since diagonal matrices commute, (106) implies the following parametrization of a generic density matrix $\rho_n \in \mathcal{D}_n$:

$$\rho_n = U_n^* D_n(\lambda_1, \dots, \lambda_n) U_n = A_{n,n}^* \cdots A_{n,2}^* D_n(\lambda_1, \dots, \lambda_n) A_{n,2} \cdots A_{n,n} \quad (129)$$

where the matrices $A_{n,j}$ and the matrix D_n are parametrized as described above. Recall that for each $j = 2, \dots, n$ both the parameter set $P_{n,j}$ for the matrix $A_{n,j}$ and the concrete form of this matrix have been given explicitly. The number of parameters is easily calculated: There are $n^2 - n$ real parameters for the product $A_{n,2} \cdots A_{n,n}$ and $n - 1$ parameters representing the eigenvalues $\lambda_1, \dots, \lambda_n$ subject to the normalization condition $\sum_{j=1}^n \lambda_j = 1$. This gives $n^2 - 1$ independent real parameters as in the Bloch vector parametrization.

If we introduce the set

$$\Lambda_n = \{\underline{\lambda} = (\lambda_1, \dots, \lambda_n) \in \mathbb{R}^n : \lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n \geq 0, \sum_{j=1}^n \lambda_j = 1\} \quad (130)$$

we can specify the parameter set Q_n of this parametrization as

$$Q_n = \{(\underline{\lambda}, \theta_j, z_j) : \underline{\lambda} \in \Lambda_n, \theta_j \in [0, \pi/2], z_j \in S(\mathbb{C}^{j-1}), j = 2, \dots, n\}. \quad (131)$$

Our recursion relation (125) for unitary matrices leads to an interesting recursion relation for density matrices in different dimensions. Denote the product $A_{n,2} \cdots A_{n,n-1}$ by U_{n-1} . Then, using (125), we can deduce from (129) the recursion formula

$$\rho_n = A_{n,n}^* \begin{pmatrix} U_{n-1}^* & \mathbb{O} \\ \mathbb{O} & 1 \end{pmatrix} \begin{pmatrix} D_{n-1}(\lambda_1, \dots, \lambda_{n-1}) & \mathbb{O} \\ \mathbb{O} & \lambda_n \end{pmatrix} \begin{pmatrix} U_{n-1} & \mathbb{O} \\ \mathbb{O} & 1 \end{pmatrix} A_{n,n} \quad (132)$$

$$= A_{n,n}^* \begin{pmatrix} \rho_{n-1} & \mathbb{O} \\ \mathbb{O} & \lambda_n \end{pmatrix} A_{n,n} \quad (133)$$

where

$$\rho_{n-1} = U_{n-1}^* D_{n-1}(\lambda_1, \dots, \lambda_{n-1}) U_{n-1} \quad (134)$$

is a positive matrix in dimension $n - 1$ with trace $\text{Tr} \rho_{n-1} = 1 - \lambda_n$.

While in the case of the Bloch vector parametrization the question of uniqueness was quite easy to answer, it is fairly complicated in the case of the Jarlskog parametrization and only partial answers are known. Given $\underline{\lambda} \in \Lambda_n$, consider the diagonal matrix $D_n(\underline{\lambda})$ of eigenvalues and the commutant of this matrix in $SU(n)$,

$$D_n(\underline{\lambda})' = \{V \in SU(n) : V D_n(\underline{\lambda}) = D_n(\underline{\lambda}) V\}. \quad (135)$$

Clearly this commutant depends on $\underline{\lambda} \in \Lambda_n$. As mentioned in the previous section, in the case of a non-degenerate spectrum, i.e., if $\lambda_1 > \lambda_2 > \dots > \lambda_n \geq 0$, then this commutant is easily determined

$$D_n(\underline{\lambda})' = \{V = D_n(e^{i\alpha_1}, \dots, e^{i\alpha_n}) : \sum_{j=1}^n \alpha_j = 0\}. \quad (136)$$

Next consider the case that for some $1 \leq k < n$ one has $\lambda_1 > \lambda_2 > \dots > \lambda_k > 0$ while $\lambda_j = 0$ for $j = k + 1, \dots, n$. This case can be reduced to the previous one by restricting the density matrix

to the subspace spanned by the first k eigenvectors.

In general one can not exclude degeneracy in the spectrum of a density matrix ρ_n ; then one has to consider eigenvalues λ_j with multiplicity m_j , $j = 1, 2, \dots, k$, $k < n$, $\lambda_1 > \lambda_2 > \dots > \lambda_k$, $m_1 + \dots + m_k = n$. For this kind of a spectrum the commutant (135) is

$$D_n(\underline{\lambda})' = \left\{ V = \begin{pmatrix} V_1 & \mathbb{O} & \dots & \mathbb{O} \\ \mathbb{O} & V_2 & \dots & \mathbb{O} \\ \vdots & \vdots & \dots & \vdots \\ \mathbb{O} & \mathbb{O} & \dots & V_k \end{pmatrix} : V_j \in U(m_j), \det V = \prod_{j=1}^k \det V_j = 1 \right\}. \quad (137)$$

In order to establish an injective parametrization of density matrices in this case one has to determine the Jarlskog parametrization of elements $U_n \in SU(n)$ modulo elements in $D_n(\underline{\lambda})'$. This is not yet known.

4.3. Simple examples

As has been explained in section 2, the structure of the set of Bloch vectors is complicated when $n > 2$. In order to overcome this other parametrizations can be used. To get some inspiration on how to proceed we have a new look at the Bloch-vector parametrization for $n = 2$. In the parametrization (22) we again take $\theta = 2\vartheta$ and write the relations (17) for the eigenvalues as $|\underline{\lambda}| = x_1 - x_2$ and $1 = x_1 + x_2$. Then, with the abbreviations $c = \cos \vartheta$ and $s = \sin \vartheta$, the parametrization (22) can be written as

$$\begin{pmatrix} x_1 c^2 + x_2 s^2 & (x_1 - x_2) c s e^{-i\phi} \\ (x_1 - x_2) c s e^{i\phi} & x_2 c^2 + x_1 s^2 \end{pmatrix}, \quad (x_1, x_2, \vartheta, \phi) \in \hat{Q}_2 \quad (138)$$

where the parameter set \hat{Q}_2 has the form

$$\hat{Q}_2 = \{(x_1, x_2, \vartheta, \phi) \in \mathbb{R}^4 : 0 \leq x_1, 0 \leq x_2, x_1 + x_2 = 1, 0 \leq \vartheta \leq \pi/2, 0 \leq \phi < 2\pi\}. \quad (139)$$

In this form we can recognize the parametrization (138) to be the following product of 5 matrices:

$$\begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix} \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} x_1 & 0 \\ 0 & x_2 \end{pmatrix} \begin{pmatrix} c & s \\ -s & c \end{pmatrix} \begin{pmatrix} e^{i\phi/2} & 0 \\ 0 & e^{-i\phi/2} \end{pmatrix}. \quad (140)$$

This is of the form $\rho = U^* D_2(\lambda_1, \lambda_2) U$ where the diagonal matrix of the eigenvalues $D_2(\lambda_1, \lambda_2)$ is sandwiched between a unitary matrix U and its adjoint U^* when we set $x_i = \lambda_i$. This agrees with the parametrization (129) for $n = 2$ with

$$U = A_{2,2} = \begin{pmatrix} 1 - (1 - c_2)|z_2\rangle\langle z_2| & s_2|z_2\rangle \\ -s_2\langle z_2| & c_2 \end{pmatrix}$$

when we set $z_2 \in S(\mathbb{C})$ as $z_2 = e^{-i\phi}$ and $\theta_2 = \vartheta \in [0, \pi/2]$.

Knowing the explicit form of a density matrix ρ_2 in two dimension we can easily calculate the explicit form of a density matrix on \mathbb{C}^3 by using the recursion formula (132): Given any point $(\lambda_1, \lambda_2, \lambda_3; \theta_2, z_2; \theta_3, z_3) \in Q_3$ we find

$$\rho_3 = A_{3,3}(\theta_3, z_3)^* A_{3,2}(\theta_2, z_2)^* D_3(\lambda_1, \lambda_2, \lambda_3) A_{3,2}(\theta_2, z_2) A_{3,3}(\theta_3, z_3) \quad (141)$$

$$= A_{3,3}^* \begin{pmatrix} \rho_2' & 0 \\ 0 & \lambda_3 \end{pmatrix} A_{3,3}, \quad (142)$$

where ρ'_2 is a positive matrix with trace $\text{Tr}\rho'_2 = \lambda_1 + \lambda_2$.

Clearly, this recursive construction can be continued to $n = 4, 5, \dots$

4.4. Jarlskog parametrization of density matrices for composite systems

Consider now a density operator for the composite system living in $\mathbb{C}^n \otimes \mathbb{C}^m$. It is clear that we may parametrize it as a density operator living in \mathbb{C}^{nm} . However, by doing this we lose information about the particular tensor product structure of the total Hilbert space \mathbb{C}^{nm} . To control the division into subsystems of $\mathbb{C}^{nm} = \mathbb{C}^n \otimes \mathbb{C}^m$ let us consider ρ as an $n \times n$ matrix with $m \times m$ blocks, i.e.,

$$\rho_{n,m} = \sum_{i,j=1}^n |i\rangle\langle j| \otimes \rho_{ij}, \quad (143)$$

with ρ_{ij} being $m \times m$ complex matrices. Our aim is to provide a suitable parametrization for positive block matrices. We proceed in analogy to the previous section.

For $\underline{\lambda} = (\lambda_1, \lambda_2, \dots, \lambda_{nm}) \in \Lambda_{nm}$ we denote by $D_{nm}(\underline{\lambda})$ the diagonal matrix of eigenvalues. Then for any $U_{n,m} \in SU(nm)$

$$\rho_{n,m} = U_{n,m}^* D_{nm}(\underline{\lambda}) U_{n,m} \quad (144)$$

is a density matrix in \mathbb{C}^{nm} . Again we parametrize elements $U_{n,m} \in SU(nm)$ by

$$su(nm) \ni X_1 + X_2 + \dots + X_n \longrightarrow e^{X_1} e^{X_2} \dots e^{X_n} \in SU(nm) \quad (145)$$

where now X_1 is an $n \times$ anti-hermitian block-diagonal matrix with $m \times m$ blocks, and for $j = 2, \dots, n$ X_j is an $n \times$ anti-hermitian matrix with $m \times m$ blocks defined as follows:

$$X_j = \begin{pmatrix} I_{j-1} \otimes \mathbb{O}_m & |Z_j\rangle & \mathbb{O} \\ -\langle Z_j| & \mathbb{O}_m & \mathbb{O} \\ \mathbb{O} & \mathbb{O} & I_{n-j} \otimes \mathbb{O}_m \end{pmatrix}, \quad (146)$$

where instead of the $n - 1$ column vectors z_j used in the previous section we choose now $n - 1$ column block vectors

$$|Z_j\rangle = \begin{pmatrix} Z_{1,j} \\ Z_{2,j} \\ \vdots \\ Z_{j-1,j} \end{pmatrix}, \quad (147)$$

with $Z_{i,j}$ being $m \times m$ matrices; and similarly

$$\langle Z_j| = (Z_{1,j}^*, Z_{2,j}^*, \dots, Z_{j-1,j}^*).$$

The Jarlskog matrices $A_{n,m}^j = e^{X_j}$ are now of the following form:

$$A_{n,m}^1 = \begin{pmatrix} U_1 & \mathbb{O}_m & \cdots & \mathbb{O}_m \\ \mathbb{O}_m & U_2 & \cdots & \mathbb{O}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbb{O}_m & \mathbb{O}_m & \cdots & U_n \end{pmatrix}, \quad (148)$$

where the U_k are unitary $m \times m$ matrices. For $j = 2, \dots, n$ one finds

$$A_{n,m}^j = \begin{pmatrix} V_{n,m}^j & \mathbb{O}_m & \cdots & \mathbb{O}_m \\ \mathbb{O}_m & I_m & \cdots & \mathbb{O}_m \\ \vdots & \vdots & \ddots & \vdots \\ \mathbb{O}_m & \mathbb{O}_m & \cdots & I_m \end{pmatrix}, \quad (149)$$

where the m dimensional unit matrix I_m appears $n - j$ times and where $V_{n,m}^j$ is a unitary $j \times j$ block matrix with $m \times m$ blocks, defined as follows:

$$V_{n,m}^j = \begin{pmatrix} I_{j-1} \otimes I_m - |\tilde{Z}_j\rangle[I_{j-1} \otimes (I_m - C_j)]\langle\tilde{Z}_j| & |\tilde{Z}_j\rangle S_j \\ -S_j\langle\tilde{Z}_j| & C_j \end{pmatrix}. \quad (150)$$

Here we use the following notation: $|\tilde{Z}_j\rangle$ denotes the normalized block vector

$$\tilde{Z}_j = \frac{1}{\|Z_j\|} Z_j, \quad \|Z_j\|^2 = Z_{1,j}^* Z_{1,j} + \cdots + Z_{j-1,j}^* Z_{j-1,j}, \quad (151)$$

and $I_{j-1} \otimes I_m - |\tilde{Z}_j\rangle[I_{j-1} \otimes (I_m - C_j)]\langle\tilde{Z}_j|$ stands for the $(j-1) \times (j-1)$ block matrix

$$\sum_{k,l=1}^{j-1} |k\rangle\langle l| \otimes \tilde{Z}_{k,l}^* C_j \tilde{Z}_{l,j}, \quad (152)$$

with

$$C_j = \cos \Xi_j, \quad S_j = \sin \Xi_j, \quad \Xi_j = \|Z_j\|. \quad (153)$$

Our parametrization (144) of density matrices $\rho_{n,m}$ now reads

$$\begin{aligned} \rho_{n,m} &= A_{n,m}^{n*} A_{n,m}^{n-1*} \cdots A_{n,m}^{1*} D_{nm}(\underline{\lambda}) A_{n,m}^1 \cdots A_{n,m}^{n-1} A_{n,m}^n \\ &= A_{n,m}^{n*} \cdots A_{n,m}^{2*} D_n(\Lambda_1 | \cdots | \Lambda_n) A_{n,m}^2 \cdots A_{n,m}^n, \end{aligned} \quad (154)$$

where

$$D_n(\Lambda_1 | \cdots | \Lambda_n) = A_{n,m}^{1*} D_{nm}(\underline{\lambda}) A_{n,m}^1 \quad (155)$$

is a positive block diagonal matrix with diagonal blocks

$$\Lambda_k = U_k^* D(\lambda_{km}, \dots, \lambda_{km+m-1}) U_k \quad (156)$$

which are positive $m \times m$ matrices and which satisfy the normalization condition

$$\text{Tr}(\Lambda_1 + \cdots \Lambda_n) = 1. \quad (157)$$

4.4.1. 2×2 systems

Let us consider a $2 \otimes 2$ system to illustrate our parametrization for the well-known 2-qubit states. Taking

$$\Lambda_1 = \mathbb{O}_2, \quad \Lambda_2 = \frac{1}{2}(I_2 - \sigma_z), \quad S = \sin \alpha I_2, \quad C = \cos \alpha I_2, \quad U = \sigma_z \quad (158)$$

one obtains a family of rank-1 projectors

$$P(\alpha) = \begin{pmatrix} \sin^2 \alpha & 0 & 0 & \sin \alpha \cos \alpha \\ \sin \alpha \cos \alpha & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sin \alpha \cos \alpha & 0 & 0 & \cos^2 \alpha \end{pmatrix}, \quad (159)$$

which corresponds to a pure state

$$\psi_\alpha = \sin \alpha |00\rangle + \cos \alpha |11\rangle.$$

Note that this state is separable if and only if $S = 0$ or $C = 0$. For $S = C = I_2/\sqrt{2}$, one obtains a maximally entangled state. It shows that a nontrivial rotation by α does produce quantum entanglement.

As a second example in this class let us take $S = C = I_2/\sqrt{2}$, $U = \sigma_x$ and

$$\Lambda_1 = \frac{1}{4} \begin{pmatrix} 1-p & 0 \\ 0 & 1-p \end{pmatrix}, \quad \Lambda_2 = \frac{1}{4} \begin{pmatrix} 1-p & 0 \\ 0 & 1+3p \end{pmatrix}, \quad (160)$$

with $-1/3 \leq p \leq 1$ to guarantee positivity of the matrices Λ_i . One obtains the partially transposed Werner state (85)

$$W_{\text{pt}}(-p) = \frac{1}{4} \begin{pmatrix} 1+p & 0 & 0 & 2p \\ 0 & 1-p & 0 & 0 \\ 0 & 0 & 1-p & 0 \\ 2p & 0 & 0 & 1+p \end{pmatrix}. \quad (161)$$

As has been shown earlier, this state is separable if and only if $p \leq 1/3$. The point $p = 1/3$ is not distinguished by our parametrization.

Next we consider $S = \sin \alpha I_2$ and $C = \cos \alpha I_2$ and obtain a more general two-parameter family

$$I(p, \alpha) = \frac{1}{4} I_2 \otimes I_2 + p P(\alpha) \quad (162)$$

of $2 \otimes 2$ states. This family is separable if and only if

$$p \leq \frac{1}{1 + 2 \sin(2\alpha)}.$$

This family of states can be generalized further as follows: Instead of (160) we take

$$\Lambda_1 = \begin{pmatrix} p_2 & 0 \\ 0 & p_4 \end{pmatrix}, \quad \Lambda_2 = \begin{pmatrix} p_3 & 0 \\ 0 & p_1 \end{pmatrix}, \quad (163)$$

where $p_i \geq 0$ and $p_1 + p_2 + p_3 + p_4 = 1$. Furthermore, the S and the C matrices are chosen as

$$S = \begin{pmatrix} \sin \alpha & 0 \\ 0 & \sin \beta \end{pmatrix}, \quad C = \begin{pmatrix} \cos \alpha & 0 \\ 0 & \cos \beta \end{pmatrix}, \quad \alpha, \beta \in [0, \pi/2].$$

With $U = \sigma_x$ the following family of states results ($s_\alpha = \sin \alpha$, $c_\alpha = \cos \alpha$ and similarly for s_β and c_β , $\underline{p} = (p_1, p_2, p_3, p_4)$ as above):

$$\rho(\underline{p}; \alpha, \beta) = \begin{pmatrix} p_1 c_\alpha^2 + p_2 s_\alpha^2 & 0 & 0 & (p_1 - p_2) s_\beta c_\beta \\ 0 & p_3 c_\beta^2 + p_4 s_\beta^2 & (p_3 - p_4) s_\alpha c_\alpha & 0 \\ 0 & (p_3 - p_4) s_\alpha c_\alpha & p_3 s_\beta^2 + p_4 c_\beta^2 & 0 \\ (p_1 - p_2) s_\beta c_\beta & 0 & 0 & p_1 s_\alpha^2 + p_2 c_\alpha^2 \end{pmatrix}. \quad (164)$$

By construction or by a direct calculation we see that $\rho(\underline{p}; \alpha, \beta) \geq 0$ and $\text{Tr} \rho(\underline{p}; \alpha, \beta) = 1$ for any choice of the parameters with the restrictions given above.

Note that the above family belongs to the class of $2 \otimes 2$ circulant states considered in (68). Note also that for $\alpha = \beta = \pi/4$ the family of states (164) reduces to the family of Bell diagonal states

$$\rho(\underline{p}) = \frac{1}{2} \begin{pmatrix} p_1 + p_2 & 0 & 0 & p_1 - p_2 \\ 0 & p_3 + p_4 & p_3 - p_4 & 0 \\ 0 & p_3 - p_4 & p_3 + p_4 & 0 \\ p_1 - p_2 & 0 & 0 & p_1 + p_2 \end{pmatrix}. \quad (165)$$

In (68) the separability of these states has been investigated for various values of the parameters.

4.4.2. $2 \otimes m$ systems

For $n = 2$ and $m \geq 3$ our formula (154) reads

$$\rho_{2,m} = A_{2,m}^{2*} D_2(\Lambda_1 | \Lambda_2) A_{2,m}^2, \quad A_{2,m}^2 = V_{2,m}^2 = \begin{pmatrix} \tilde{Z} C \tilde{Z}^* & \tilde{Z} S \\ -S \tilde{Z}^* & C \end{pmatrix} \quad (166)$$

with $\tilde{Z} = U \in U(m)$ and $C = \cos \Xi_2$ and $S = \sin \Xi_2$. $D_2(\Lambda_1 | \Lambda_2)$ is given by (155), (156), and (157). Matrix multiplication gives

$$\rho_{2,m} = \begin{pmatrix} U^* & \mathbb{O}_m \\ \mathbb{O}_m & I_m \end{pmatrix} \begin{pmatrix} C U^* \Lambda_1 U C + S \Lambda_2 S & S \Lambda_2 C - C U^* \Lambda_1 U S \\ C \Lambda_2 S - S U^* \Lambda_1 U C & C \Lambda_2 C + S U^* \Lambda_1 U S \end{pmatrix} \begin{pmatrix} U & \mathbb{O}_m \\ \mathbb{O}_m & I_m \end{pmatrix} \quad (167)$$

By choosing particular values for the parameters appearing in (167) we find some examples which have been considered in the literature.

For $S = \mathbb{O}$ or $C = \mathbb{O}$ one obtains a class of block diagonal matrices

$$\begin{pmatrix} \Lambda_1 & \mathbb{O}_m \\ \mathbb{O}_m & \Lambda_2 \end{pmatrix} \quad \text{or} \quad \begin{pmatrix} \Lambda_2 & \mathbb{O}_m \\ \mathbb{O}_m & \Lambda_1 \end{pmatrix}. \quad (168)$$

These matrices represent separable $2 \otimes m$ states and thus show that quantum entanglement arises only for nontrivial Ξ_2 such that $C \neq \mathbb{O}$ and $S \neq \mathbb{O}$.

Next consider the case $\Lambda_1 = \Lambda_2 = \Lambda$ and $[\Lambda, U] = 0$. We get the following class of $2 \otimes m$ states:

$$\begin{pmatrix} U^* & \mathbb{O}_m \\ \mathbb{O}_m & I_m \end{pmatrix} \begin{pmatrix} A & B \\ B^* & A \end{pmatrix} \begin{pmatrix} U & \mathbb{O}_m \\ \mathbb{O}_m & I_m \end{pmatrix} \quad (169)$$

with

$$A = C\Lambda C + S\Lambda S, \quad B = S\Lambda C = C\Lambda S.$$

If in addition $U^*AU = A$ is assumed one gets the matrices

$$\begin{pmatrix} A & UB \\ (UB)^* & A \end{pmatrix}. \quad (170)$$

These are block Toeplitz positive matrices and it is well-known that they are separable (69). Thus (170) defines a huge family of bipartite separable states.

Similarly, the block Hankel positive matrices of (69) can be reconstructed. To this end we assume that the matrices U, Λ_1, Λ_2 and Ξ_2 satisfy

$$[U^*\Lambda_1U, \Xi_2] = 0, \quad [\Lambda_2, \Xi_2] = 0.$$

This produces the following class of $2 \otimes m$ states:

$$\begin{pmatrix} U^* & \mathbb{O}_m \\ \mathbb{O}_m & I_m \end{pmatrix} \begin{pmatrix} A_1 & B' \\ B' & A_2 \end{pmatrix} \begin{pmatrix} U & \mathbb{O}_m \\ \mathbb{O}_m & I_m \end{pmatrix} \quad (171)$$

with $A_i = C\Lambda_iC + S\Lambda_iS$ and $B' = SC(\Lambda_2 - U^*\Lambda_1U)$. Under the additional assumption $UB' = B'U$ we arrive at matrices of the form

$$\begin{pmatrix} U^*A_1U & X \\ X & A_2 \end{pmatrix} \quad (172)$$

with $X = UB'$. These are block Hankel positive matrices and hence separable (69).

5. Conclusion

In this review we have discussed different parametrizations of $n \times n$ density matrices. We have compared three different parametrizations, namely the Bloch vector, coset, and Jarlskog parametrizations. Of these the Bloch vector parametrization is the oldest and most widely used, while the two others are relatively recent discoveries and consequently not so well known.

The Bloch vector parametrization has found more applications in physical problems than any other density matrix parametrization. This is due to the inherent simplicity of the parametrization. The basis matrices used in this representation are hermitian, which guarantees that the components of the Bloch vector are real. Furthermore, these components can be obtained straightforwardly as expectation values of hermitian operators. Therefore, given a density operator, the calculation of the components of the corresponding Bloch vector can be done straightforwardly. On the other hand, there is a serious disadvantage in the Bloch vector parametrization: In all the cases of $n \geq 3$ it is practically impossible to determine the parameter set corresponding to physical states explicitly (see Section 2.2). Only for a two-level system the parameter set is easily determined and is given by unit ball in \mathbb{R}^3 , the so called Bloch ball. The difficulty derives

from the requirement that a density matrix has to be a positive operator. As yet, there is no simple way to determine which Bloch vectors lead to positive matrices. Despite the complexity of the parameter set, the Bloch vector parametrization has many applications. It has been known for a long time that it gives a bijective mapping between the states of a two-level system and the points of the Bloch ball, providing an elegant way to visualize the states and dynamics of two-level systems. Another advantage is that the hermiticity of the basis enables to write the density matrices and Hamiltonian in the same basis. This makes possible to derive easily the differential equation giving the time-evolution of the Bloch vector. Under some conditions for the Hamiltonian of the system, this approach allows to identify various constants of motion. The Bloch vector has turned out to be useful also when the entanglement and separability of two-qubit states is examined.

The second parametrization discussed in detail in this article is the Jarlskog parametrization which is based on a suitable parametrization of (special) unitary matrices. Its main advantages are (see sections 4.2 and 5.1):

- Its parameter set is given explicitly;
- it is recursive;
- it extends naturally to composite systems.

However, in the form presented here, it contains redundancy in the case of a degenerate spectrum. We have indicated how to eliminate this and get injectivity for this parametrization, too.

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